



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:46 AM EDT

PDB ID : 4AIP / pdb_00004aip
Title : The FrpB iron transporter from Neisseria meningitidis (F3-3 variant)
Authors : Saleem, M.; Prince, S.M.; Derrick, J.P.
Deposited on : 2012-02-11
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

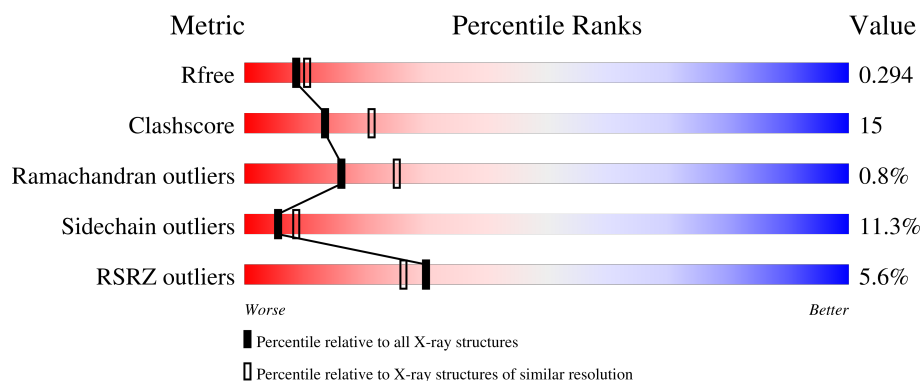
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	742	5% 60% 22% 6% • 11%
1	B	742	4% 61% 22% 6% • 10%
1	C	742	6% 60% 23% 6% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15985 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FE-REGULATED PROTEIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5178	3234	944	995	5			
1	B	665	Total	C	N	O	S	0	0	0
			5209	3247	956	1002	4			
1	C	665	Total	C	N	O	S	0	0	0
			5212	3253	952	1002	5			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q51162
A	2	HIS	-	expression tag	UNP Q51162
A	3	HIS	-	expression tag	UNP Q51162
A	4	HIS	-	expression tag	UNP Q51162
A	5	HIS	-	expression tag	UNP Q51162
A	6	HIS	-	expression tag	UNP Q51162
A	7	HIS	-	expression tag	UNP Q51162
A	8	SER	-	expression tag	UNP Q51162
A	9	SER	-	expression tag	UNP Q51162
A	10	GLY	-	expression tag	UNP Q51162
A	11	LEU	-	expression tag	UNP Q51162
A	12	VAL	-	expression tag	UNP Q51162
A	13	PRO	-	expression tag	UNP Q51162
A	14	ARG	-	expression tag	UNP Q51162
A	15	GLY	-	expression tag	UNP Q51162
A	16	SER	-	expression tag	UNP Q51162
A	17	GLY	-	expression tag	UNP Q51162
A	18	MET	-	expression tag	UNP Q51162
A	19	LYS	-	expression tag	UNP Q51162
A	20	GLU	-	expression tag	UNP Q51162
A	21	THR	-	expression tag	UNP Q51162
A	22	ALA	-	expression tag	UNP Q51162
A	23	ALA	-	expression tag	UNP Q51162

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	-	expression tag	UNP Q51162
A	25	LYS	-	expression tag	UNP Q51162
A	26	PHE	-	expression tag	UNP Q51162
A	27	GLU	-	expression tag	UNP Q51162
A	28	ARG	-	expression tag	UNP Q51162
A	29	GLN	-	expression tag	UNP Q51162
A	30	HIS	-	expression tag	UNP Q51162
A	31	MET	-	expression tag	UNP Q51162
A	32	ASP	-	expression tag	UNP Q51162
A	33	SER	-	expression tag	UNP Q51162
A	34	PRO	-	expression tag	UNP Q51162
A	35	ASP	-	expression tag	UNP Q51162
A	36	LEU	-	expression tag	UNP Q51162
A	37	GLY	-	expression tag	UNP Q51162
A	38	THR	-	expression tag	UNP Q51162
A	39	ASP	-	expression tag	UNP Q51162
A	40	ASP	-	expression tag	UNP Q51162
A	41	ASP	-	expression tag	UNP Q51162
A	42	ASP	-	expression tag	UNP Q51162
A	43	LYS	-	expression tag	UNP Q51162
A	44	MET	-	expression tag	UNP Q51162
A	197	ASN	GLU	conflict	UNP Q51162
A	446	ILE	VAL	conflict	UNP Q51162
B	1	MET	-	expression tag	UNP Q51162
B	2	HIS	-	expression tag	UNP Q51162
B	3	HIS	-	expression tag	UNP Q51162
B	4	HIS	-	expression tag	UNP Q51162
B	5	HIS	-	expression tag	UNP Q51162
B	6	HIS	-	expression tag	UNP Q51162
B	7	HIS	-	expression tag	UNP Q51162
B	8	SER	-	expression tag	UNP Q51162
B	9	SER	-	expression tag	UNP Q51162
B	10	GLY	-	expression tag	UNP Q51162
B	11	LEU	-	expression tag	UNP Q51162
B	12	VAL	-	expression tag	UNP Q51162
B	13	PRO	-	expression tag	UNP Q51162
B	14	ARG	-	expression tag	UNP Q51162
B	15	GLY	-	expression tag	UNP Q51162
B	16	SER	-	expression tag	UNP Q51162
B	17	GLY	-	expression tag	UNP Q51162
B	18	MET	-	expression tag	UNP Q51162
B	19	LYS	-	expression tag	UNP Q51162

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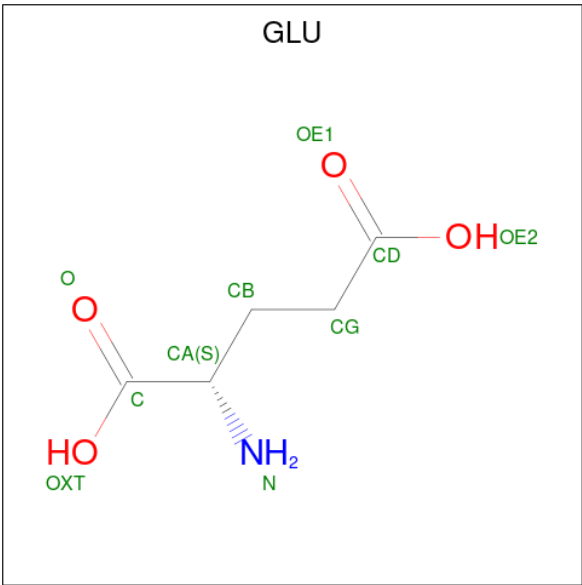
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	GLU	-	expression tag	UNP Q51162
B	21	THR	-	expression tag	UNP Q51162
B	22	ALA	-	expression tag	UNP Q51162
B	23	ALA	-	expression tag	UNP Q51162
B	24	ALA	-	expression tag	UNP Q51162
B	25	LYS	-	expression tag	UNP Q51162
B	26	PHE	-	expression tag	UNP Q51162
B	27	GLU	-	expression tag	UNP Q51162
B	28	ARG	-	expression tag	UNP Q51162
B	29	GLN	-	expression tag	UNP Q51162
B	30	HIS	-	expression tag	UNP Q51162
B	31	MET	-	expression tag	UNP Q51162
B	32	ASP	-	expression tag	UNP Q51162
B	33	SER	-	expression tag	UNP Q51162
B	34	PRO	-	expression tag	UNP Q51162
B	35	ASP	-	expression tag	UNP Q51162
B	36	LEU	-	expression tag	UNP Q51162
B	37	GLY	-	expression tag	UNP Q51162
B	38	THR	-	expression tag	UNP Q51162
B	39	ASP	-	expression tag	UNP Q51162
B	40	ASP	-	expression tag	UNP Q51162
B	41	ASP	-	expression tag	UNP Q51162
B	42	ASP	-	expression tag	UNP Q51162
B	43	LYS	-	expression tag	UNP Q51162
B	44	MET	-	expression tag	UNP Q51162
B	197	ASN	GLU	conflict	UNP Q51162
B	446	ILE	VAL	conflict	UNP Q51162
C	1	MET	-	expression tag	UNP Q51162
C	2	HIS	-	expression tag	UNP Q51162
C	3	HIS	-	expression tag	UNP Q51162
C	4	HIS	-	expression tag	UNP Q51162
C	5	HIS	-	expression tag	UNP Q51162
C	6	HIS	-	expression tag	UNP Q51162
C	7	HIS	-	expression tag	UNP Q51162
C	8	SER	-	expression tag	UNP Q51162
C	9	SER	-	expression tag	UNP Q51162
C	10	GLY	-	expression tag	UNP Q51162
C	11	LEU	-	expression tag	UNP Q51162
C	12	VAL	-	expression tag	UNP Q51162
C	13	PRO	-	expression tag	UNP Q51162
C	14	ARG	-	expression tag	UNP Q51162
C	15	GLY	-	expression tag	UNP Q51162

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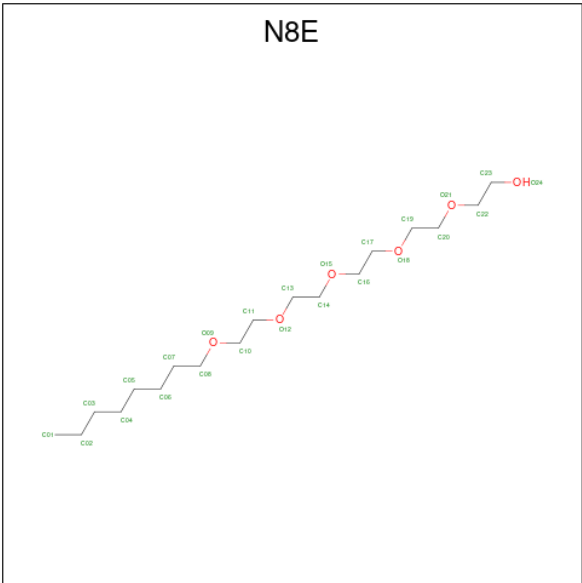
Chain	Residue	Modelled	Actual	Comment	Reference
C	16	SER	-	expression tag	UNP Q51162
C	17	GLY	-	expression tag	UNP Q51162
C	18	MET	-	expression tag	UNP Q51162
C	19	LYS	-	expression tag	UNP Q51162
C	20	GLU	-	expression tag	UNP Q51162
C	21	THR	-	expression tag	UNP Q51162
C	22	ALA	-	expression tag	UNP Q51162
C	23	ALA	-	expression tag	UNP Q51162
C	24	ALA	-	expression tag	UNP Q51162
C	25	LYS	-	expression tag	UNP Q51162
C	26	PHE	-	expression tag	UNP Q51162
C	27	GLU	-	expression tag	UNP Q51162
C	28	ARG	-	expression tag	UNP Q51162
C	29	GLN	-	expression tag	UNP Q51162
C	30	HIS	-	expression tag	UNP Q51162
C	31	MET	-	expression tag	UNP Q51162
C	32	ASP	-	expression tag	UNP Q51162
C	33	SER	-	expression tag	UNP Q51162
C	34	PRO	-	expression tag	UNP Q51162
C	35	ASP	-	expression tag	UNP Q51162
C	36	LEU	-	expression tag	UNP Q51162
C	37	GLY	-	expression tag	UNP Q51162
C	38	THR	-	expression tag	UNP Q51162
C	39	ASP	-	expression tag	UNP Q51162
C	40	ASP	-	expression tag	UNP Q51162
C	41	ASP	-	expression tag	UNP Q51162
C	42	ASP	-	expression tag	UNP Q51162
C	43	LYS	-	expression tag	UNP Q51162
C	44	MET	-	expression tag	UNP Q51162
C	197	ASN	GLU	conflict	UNP Q51162
C	446	ILE	VAL	conflict	UNP Q51162

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (CCD ID: N8E) (formula: C₁₈H₃₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			24	18	6		
3	B	1	Total	C	O	0	0
			24	18	6		

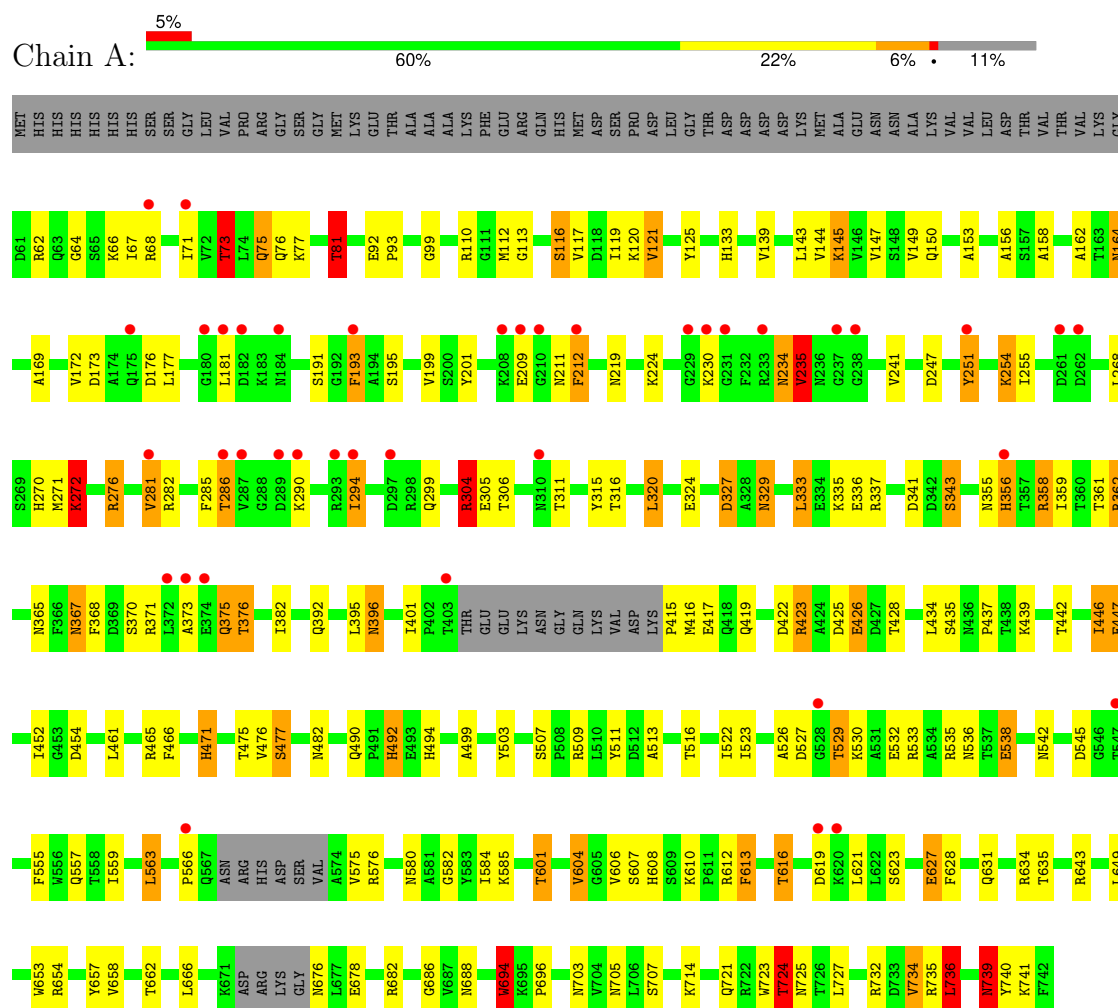
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total 133	O 133	0	0
4	B	80	Total 80	O 80	0	0
4	C	115	Total 115	O 115	0	0

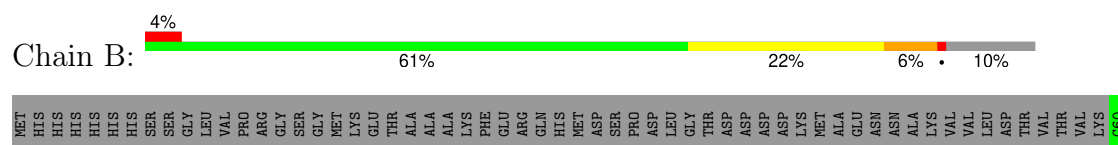
3 Residue-property plots

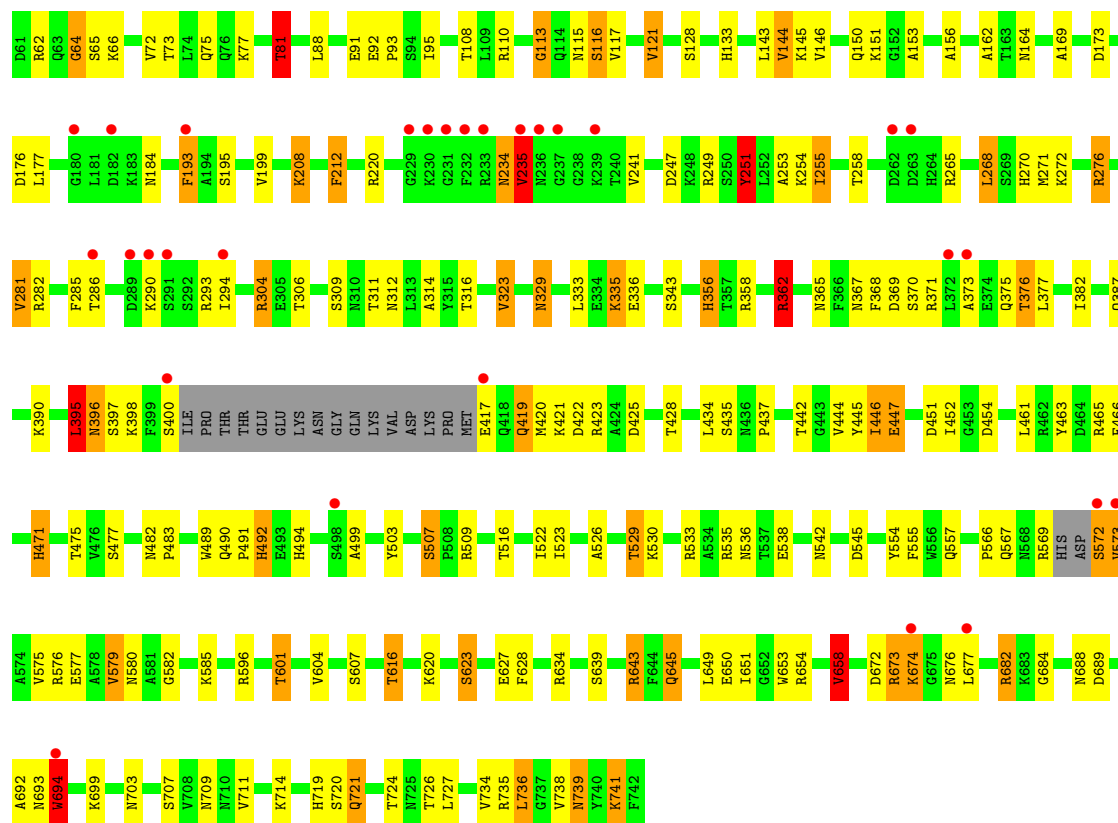
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: FE-REGULATED PROTEIN B

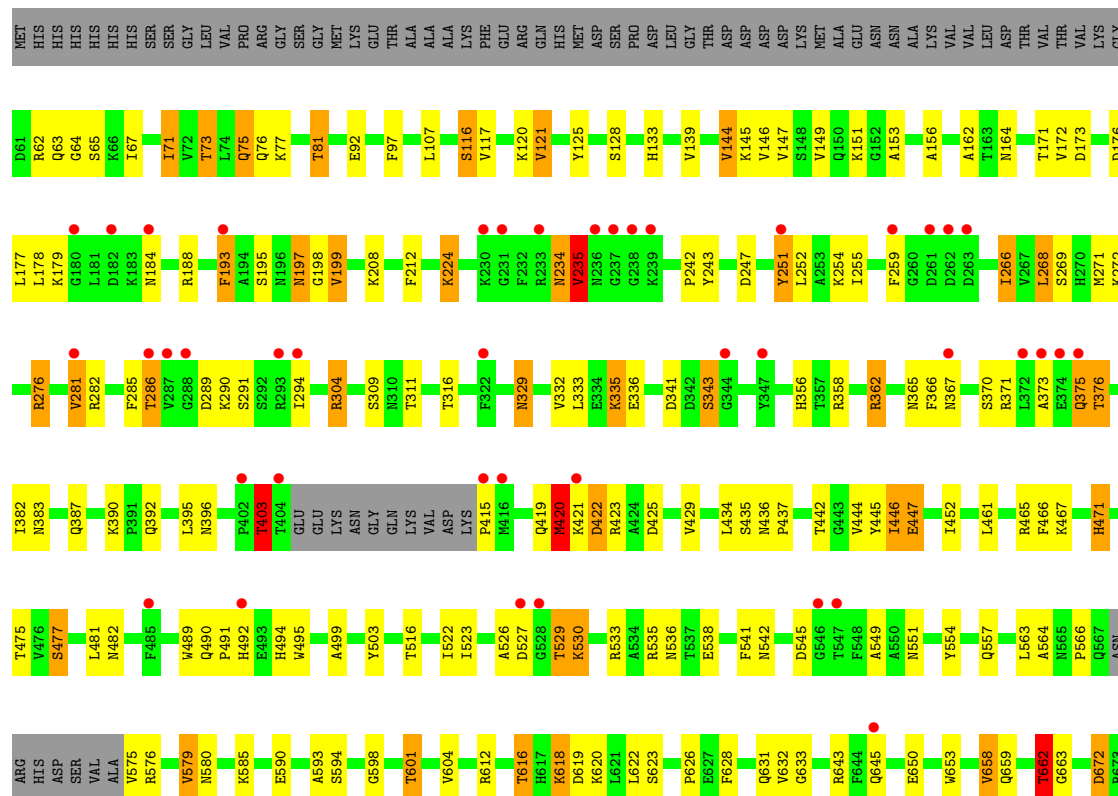


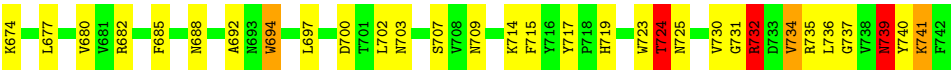
• Molecule 1: FE-REGULATED PROTEIN B





• Molecule 1: FE-REGULATED PROTEIN B





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.32Å 104.62Å 269.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.55 – 2.40 134.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.4 (134.55-2.40) 90.4 (134.55-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.242 , 0.296 0.242 , 0.294	Depositor DCC
R_{free} test set	4316 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15985	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: N8E

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.39	28/5286 (0.5%)	1.31	40/7135 (0.6%)
1	B	1.31	17/5316 (0.3%)	1.26	36/7173 (0.5%)
1	C	1.39	29/5321 (0.5%)	1.34	41/7182 (0.6%)
All	All	1.36	74/15923 (0.5%)	1.30	117/21490 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	193	PHE	CB-CG	-11.67	1.23	1.50
1	A	212	PHE	CG-CD1	-10.78	1.16	1.38
1	A	212	PHE	CB-CG	-10.31	1.26	1.50
1	C	193	PHE	CA-C	-10.08	1.40	1.52
1	A	358	ARG	CZ-NH2	-8.93	1.21	1.33
1	A	212	PHE	CE2-CZ	-8.61	1.12	1.38
1	C	62	ARG	CZ-NH1	-8.26	1.21	1.32
1	C	193	PHE	CE1-CZ	-8.23	1.14	1.38
1	A	304	ARG	CZ-NH1	-7.82	1.21	1.32
1	C	663	GLY	N-CA	7.67	1.53	1.45
1	B	193	PHE	CB-CG	-7.66	1.33	1.50
1	A	73	THR	CB-CG2	-7.30	1.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	PHE	CB-CG	-7.26	1.33	1.50
1	A	193	PHE	N-CA	-7.18	1.37	1.46
1	B	212	PHE	CB-CG	-7.09	1.34	1.50
1	A	119	ILE	CA-CB	6.72	1.62	1.54
1	A	601	THR	CA-CB	6.72	1.64	1.53
1	C	212	PHE	CB-CG	-6.67	1.35	1.50
1	A	327	ASP	CA-C	-6.48	1.44	1.52
1	C	147	VAL	CA-CB	-6.45	1.46	1.54
1	B	73	THR	CB-CG2	-6.43	1.31	1.52
1	C	193	PHE	CG-CD1	-6.40	1.25	1.38
1	B	463	TYR	N-CA	-6.37	1.38	1.46
1	C	356	HIS	CB-CG	-6.31	1.41	1.50
1	B	658	VAL	CA-CB	6.16	1.61	1.54
1	C	356	HIS	CA-C	-6.12	1.45	1.52
1	B	362	ARG	CZ-NH1	-6.09	1.24	1.32
1	C	62	ARG	CZ-NH2	-6.08	1.25	1.33
1	C	444	VAL	CA-CB	6.00	1.64	1.55
1	B	601	THR	CA-CB	5.98	1.63	1.53
1	B	208	LYS	CA-C	5.95	1.59	1.52
1	C	73	THR	CB-CG2	-5.87	1.33	1.52
1	A	254	LYS	CB-CG	-5.86	1.34	1.52
1	C	601	THR	CA-CB	5.83	1.63	1.53
1	B	358	ARG	CZ-NH2	-5.80	1.25	1.33
1	B	251	TYR	CB-CG	-5.75	1.39	1.51
1	C	252	LEU	N-CA	-5.71	1.39	1.46
1	C	375	GLN	CG-CD	-5.70	1.37	1.52
1	A	375	GLN	CG-CD	-5.65	1.38	1.52
1	A	212	PHE	CG-CD2	-5.63	1.27	1.38
1	A	355	ASN	N-CA	-5.59	1.39	1.46
1	C	358	ARG	CZ-NH2	-5.59	1.26	1.33
1	C	193	PHE	CG-CD2	-5.57	1.27	1.38
1	B	573	VAL	CA-CB	5.57	1.62	1.54
1	C	467	LYS	N-CA	-5.57	1.39	1.46
1	C	383	ASN	CA-C	-5.57	1.45	1.52
1	A	563	LEU	CA-C	-5.43	1.46	1.52
1	B	738	VAL	CA-CB	5.40	1.61	1.54
1	B	314	ALA	CA-C	-5.39	1.46	1.52
1	A	315	TYR	C-O	-5.39	1.17	1.24
1	A	147	VAL	CA-CB	-5.37	1.47	1.54
1	C	366	PHE	CA-C	-5.36	1.45	1.52
1	A	254	LYS	CE-NZ	-5.34	1.33	1.49
1	B	212	PHE	CG-CD2	-5.32	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466	PHE	N-CA	-5.29	1.39	1.45
1	B	375	GLN	CG-CD	-5.28	1.38	1.52
1	A	62	ARG	CZ-NH2	-5.25	1.26	1.33
1	C	709	ASN	CA-C	-5.25	1.46	1.52
1	C	356	HIS	CA-CB	-5.24	1.41	1.53
1	A	439	LYS	N-CA	-5.23	1.39	1.46
1	A	286	THR	CB-CG2	-5.22	1.35	1.52
1	B	62	ARG	CZ-NH1	-5.15	1.25	1.32
1	C	212	PHE	CG-CD1	-5.14	1.28	1.38
1	C	739	ASN	CA-C	-5.12	1.46	1.52
1	A	627	GLU	CA-C	5.11	1.59	1.52
1	C	212	PHE	CG-CD2	-5.09	1.28	1.38
1	C	269	SER	CA-C	5.07	1.58	1.52
1	C	336	GLU	CA-C	-5.06	1.46	1.52
1	A	476	VAL	C-O	-5.05	1.19	1.24
1	A	212	PHE	CD1-CE1	-5.03	1.23	1.38
1	C	198	GLY	C-O	-5.02	1.18	1.23
1	A	367	ASN	CB-CG	-5.02	1.39	1.52
1	A	193	PHE	CD1-CE1	-5.01	1.23	1.38
1	A	193	PHE	CD2-CE2	-5.00	1.23	1.38

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	ARG	NE-CZ-NH2	12.54	130.48	119.20
1	C	662	THR	CA-C-N	-11.78	110.61	122.27
1	C	662	THR	C-N-CA	-11.78	110.61	122.27
1	B	362	ARG	NE-CZ-NH2	10.61	128.75	119.20
1	A	724	THR	CA-C-N	-10.07	107.42	123.23
1	A	724	THR	C-N-CA	-10.07	107.42	123.23
1	B	281	VAL	N-CA-C	-9.45	96.61	109.37
1	C	663	GLY	N-CA-C	9.42	126.54	112.41
1	C	356	HIS	CB-CA-C	-9.11	91.98	109.37
1	A	304	ARG	NE-CZ-NH1	-9.09	112.42	121.50
1	A	212	PHE	CB-CA-C	8.49	128.74	110.07
1	C	281	VAL	N-CA-C	-8.32	98.14	109.37
1	A	281	VAL	N-CA-C	-8.27	98.20	109.37
1	A	736	LEU	CA-C-N	8.05	127.74	122.18
1	A	736	LEU	C-N-CA	8.05	127.74	122.18
1	C	234	ASN	N-CA-C	7.90	123.12	113.17
1	C	304	ARG	NE-CZ-NH2	7.78	126.20	119.20
1	B	724	THR	CA-C-N	-7.62	110.73	122.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	724	THR	C-N-CA	-7.62	110.73	122.16
1	C	724	THR	CA-C-N	-7.49	112.43	122.85
1	C	724	THR	C-N-CA	-7.49	112.43	122.85
1	C	62	ARG	NE-CZ-NH2	7.31	125.78	119.20
1	C	193	PHE	CB-CA-C	-7.29	95.44	109.37
1	A	234	ASN	N-CA-C	6.94	121.91	113.17
1	A	446	ILE	CB-CA-C	-6.94	98.47	111.30
1	B	356	HIS	N-CA-CB	-6.90	99.52	110.77
1	B	446	ILE	CB-CA-C	-6.79	98.56	110.71
1	C	446	ILE	CB-CA-C	-6.70	99.13	110.71
1	A	694	TRP	N-CA-C	6.54	120.05	109.40
1	A	375	GLN	CB-CA-C	-6.38	99.39	110.17
1	C	62	ARG	NH1-CZ-NH2	-6.36	111.03	119.30
1	C	672	ASP	N-CA-C	6.34	118.65	109.71
1	C	620	LYS	N-CA-C	-6.29	99.77	109.76
1	A	329	ASN	N-CA-C	-6.28	98.38	108.55
1	B	395	LEU	N-CA-C	6.20	122.43	114.56
1	C	73	THR	OG1-CB-CG2	-6.16	96.99	109.30
1	B	724	THR	N-CA-C	-6.14	102.57	110.19
1	A	62	ARG	NH1-CZ-NH2	-6.10	111.38	119.30
1	C	335	LYS	CD-CE-NZ	6.09	131.39	111.90
1	B	234	ASN	N-CA-C	6.04	120.78	113.17
1	B	362	ARG	NE-CZ-NH1	-6.03	115.47	121.50
1	C	403	THR	N-CA-C	-6.00	104.83	111.36
1	A	362	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	C	662	THR	N-CA-C	5.92	120.23	112.13
1	C	304	ARG	NE-CZ-NH1	-5.92	115.58	121.50
1	B	304	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	C	619	ASP	CA-C-N	-5.89	113.08	121.50
1	C	619	ASP	C-N-CA	-5.89	113.08	121.50
1	A	358	ARG	NE-CZ-NH1	5.85	127.35	121.50
1	C	490	GLN	CA-C-N	5.85	125.39	119.19
1	C	490	GLN	C-N-CA	5.85	125.39	119.19
1	C	362	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	C	579	VAL	CB-CA-C	-5.80	101.73	110.55
1	B	694	TRP	CA-CB-CG	5.79	124.60	113.60
1	A	230	LYS	N-CA-C	5.75	118.67	110.10
1	B	375	GLN	CB-CA-C	-5.74	99.66	109.65
1	A	81	THR	N-CA-C	-5.73	105.01	113.61
1	C	193	PHE	CG-CD1-CE1	5.71	130.40	120.70
1	B	329	ASN	N-CA-C	-5.69	98.99	108.32
1	B	254	LYS	CD-CE-NZ	5.69	130.10	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	ARG	N-CA-C	5.63	118.40	109.50
1	A	371	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	A	601	THR	CB-CA-C	5.62	119.14	110.14
1	B	371	ARG	NE-CZ-NH1	-5.57	115.94	121.50
1	A	538	GLU	N-CA-C	5.56	117.29	108.79
1	C	527	ASP	N-CA-C	5.54	117.32	111.28
1	B	719	HIS	N-CA-C	5.50	119.16	112.23
1	A	575	VAL	N-CA-C	-5.48	100.23	108.12
1	A	396	ASN	N-CA-CB	-5.48	101.23	110.49
1	A	272	LYS	CB-CG-CD	5.46	123.85	111.30
1	C	371	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	C	694	TRP	CA-CB-CG	5.44	123.94	113.60
1	B	304	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	B	694	TRP	N-CA-C	5.41	118.22	109.40
1	A	139	VAL	CA-C-N	5.41	129.13	121.61
1	A	139	VAL	C-N-CA	5.41	129.13	121.61
1	B	492	HIS	N-CA-C	-5.41	101.08	109.24
1	A	320	LEU	N-CA-C	-5.38	106.59	112.72
1	B	674	LYS	N-CA-C	-5.37	106.86	113.41
1	A	294	ILE	CB-CG1-CD1	-5.37	102.53	113.80
1	B	362	ARG	CA-C-N	-5.31	115.88	121.35
1	B	362	ARG	C-N-CA	-5.31	115.88	121.35
1	B	451	ASP	CB-CA-C	-5.31	102.29	110.78
1	A	356	HIS	CB-CA-C	5.29	120.13	109.38
1	A	694	TRP	CA-CB-CG	5.27	123.62	113.60
1	A	739	ASN	CB-CA-C	-5.26	98.97	109.33
1	A	492	HIS	N-CA-C	-5.25	101.31	109.24
1	B	73	THR	OG1-CB-CG2	-5.24	98.82	109.30
1	B	490	GLN	CA-C-N	5.22	124.72	119.19
1	B	490	GLN	C-N-CA	5.22	124.72	119.19
1	C	193	PHE	CB-CG-CD2	5.21	129.55	120.70
1	B	721	GLN	N-CA-C	-5.19	99.75	110.80
1	B	113	GLY	N-CA-C	5.19	121.06	112.66
1	C	329	ASN	N-CA-C	-5.18	99.83	108.32
1	B	444	VAL	N-CA-C	-5.17	100.88	108.85
1	C	375	GLN	CB-CA-C	-5.17	101.45	110.09
1	C	732	ARG	N-CA-CB	-5.17	101.47	109.69
1	A	428	THR	CB-CA-C	-5.15	102.77	110.90
1	C	371	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	C	197	ASN	N-CA-C	-5.14	96.62	111.00
1	B	81	THR	N-CA-C	-5.12	106.43	113.30
1	B	454	ASP	CB-CA-C	5.12	119.37	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	TYR	CE1-CZ-OH	-5.12	104.54	119.90
1	C	358	ARG	N-CA-C	5.12	117.74	109.40
1	A	211	ASN	CA-C-N	-5.10	113.95	122.21
1	A	211	ASN	C-N-CA	-5.10	113.95	122.21
1	A	527	ASP	N-CA-C	5.10	116.84	111.28
1	C	741	LYS	CA-CB-CG	5.09	124.28	114.10
1	A	739	ASN	N-CA-CB	5.08	119.78	111.08
1	B	736	LEU	CA-C-N	5.08	125.69	122.18
1	B	736	LEU	C-N-CA	5.08	125.69	122.18
1	B	390	LYS	CA-C-N	-5.07	115.34	120.21
1	B	390	LYS	C-N-CA	-5.07	115.34	120.21
1	C	626	PRO	CA-C-N	5.07	128.42	120.82
1	C	626	PRO	C-N-CA	5.07	128.42	120.82
1	A	604	VAL	CB-CA-C	-5.04	101.78	110.30
1	C	71	ILE	CB-CA-C	-5.01	105.37	112.14

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	395	LEU	Peptide
1	B	395	LEU	Peptide
1	C	395	LEU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5178	0	5017	169	0
1	B	5209	0	5045	154	0
1	C	5212	0	5053	164	0
2	A	10	0	5	1	0
3	A	24	0	38	4	0
3	B	24	0	38	14	0
4	A	133	0	0	12	0
4	B	80	0	0	7	0
4	C	115	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15985	0	15196	458	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (458) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLU:OE1	1:C:740:TYR:CE1	1.90	1.24
1:A:285:PHE:CB	1:A:294:ILE:HD11	1.75	1.16
1:A:209:GLU:OE1	1:C:740:TYR:CZ	1.97	1.15
1:C:732:ARG:CG	1:C:732:ARG:HH11	1.62	1.08
1:B:285:PHE:CB	1:B:294:ILE:HD11	1.83	1.07
1:B:285:PHE:HB3	1:B:294:ILE:CD1	1.85	1.06
1:C:367:ASN:OD1	1:C:445:TYR:OH	1.74	1.04
1:C:285:PHE:CB	1:C:294:ILE:HD11	1.88	1.03
1:C:285:PHE:HB3	1:C:294:ILE:CD1	1.89	1.03
1:C:242:PRO:O	1:C:286:THR:HG22	1.62	1.00
1:C:732:ARG:HH11	1:C:732:ARG:HG2	1.28	0.98
1:A:285:PHE:HB3	1:A:294:ILE:HD11	0.99	0.97
1:A:193:PHE:CE1	1:B:311:THR:HG21	1.99	0.97
1:A:285:PHE:HB3	1:A:294:ILE:CD1	1.94	0.96
1:C:304:ARG:HD2	4:C:2079:HOH:O	1.64	0.95
1:B:362:ARG:HG3	1:B:362:ARG:HH11	1.32	0.94
1:B:362:ARG:HH11	1:B:362:ARG:CG	1.77	0.94
1:B:736:LEU:CD2	1:C:268:LEU:HD11	1.99	0.93
1:C:732:ARG:CG	1:C:732:ARG:NH1	2.25	0.92
1:C:177:LEU:O	1:C:741:LYS:HE3	1.70	0.92
1:C:612:ARG:HH12	1:C:631:GLN:NE2	1.68	0.92
1:B:255:ILE:HB	3:B:1743:N8E:H141	1.53	0.91
1:B:645:GLN:OE1	1:B:645:GLN:HA	1.70	0.90
1:B:81:THR:HG23	1:B:735:ARG:HD3	1.53	0.89
1:C:281:VAL:O	1:C:282:ARG:HB2	1.74	0.88
1:A:423:ARG:HH11	1:A:423:ARG:HG3	1.37	0.87
1:C:285:PHE:HB3	1:C:294:ILE:HD11	0.94	0.87
1:C:471:HIS:HE1	1:C:523:ILE:H	1.23	0.86
1:B:281:VAL:O	1:B:282:ARG:HB2	1.76	0.85
1:A:471:HIS:HE1	1:A:523:ILE:H	1.24	0.85
1:B:471:HIS:HE1	1:B:523:ILE:H	1.22	0.84
1:B:396:ASN:HD21	1:B:434:LEU:HG	1.40	0.84
1:C:64:GLY:H	1:C:542:ASN:HD21	1.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:THR:HG22	4:C:2102:HOH:O	1.77	0.83
1:C:653:TRP:HE1	1:C:688:ASN:HD22	1.21	0.83
1:C:612:ARG:HH12	1:C:631:GLN:HE21	1.27	0.82
1:C:732:ARG:NH1	1:C:732:ARG:HG3	1.91	0.82
1:B:285:PHE:HB3	1:B:294:ILE:HD11	0.90	0.81
1:A:423:ARG:NH1	1:A:426:GLU:OE2	2.14	0.81
1:B:703:ASN:HD22	1:B:739:ASN:HD21	1.29	0.81
1:A:268:LEU:HD22	1:C:193:PHE:CE2	2.15	0.80
1:C:242:PRO:O	1:C:286:THR:CG2	2.30	0.80
1:B:736:LEU:HD23	1:C:268:LEU:HD11	1.64	0.79
1:B:367:ASN:OD1	1:B:445:TYR:OH	1.99	0.79
1:A:81:THR:HG23	1:A:735:ARG:HD3	1.62	0.79
1:A:281:VAL:O	1:A:282:ARG:HB2	1.82	0.79
1:B:672:ASP:O	1:B:674:LYS:N	2.15	0.79
1:B:212:PHE:HB3	3:B:1743:N8E:H231	1.67	0.76
1:A:530:LYS:H	1:A:580:ASN:HD21	1.32	0.76
1:A:64:GLY:H	1:A:542:ASN:HD21	1.31	0.75
1:C:471:HIS:CE1	1:C:523:ILE:H	2.05	0.75
1:A:423:ARG:HG3	1:A:423:ARG:NH1	2.01	0.75
1:A:201:TYR:HE1	3:B:1743:N8E:H013	1.52	0.74
1:A:703:ASN:HD22	1:A:739:ASN:ND2	1.85	0.74
1:B:672:ASP:C	1:B:674:LYS:H	1.95	0.74
1:C:419:GLN:O	1:C:422:ASP:HB2	1.87	0.74
1:A:471:HIS:CE1	1:A:523:ILE:H	2.05	0.73
1:B:251:TYR:HE1	1:B:272:LYS:HD2	1.53	0.72
1:B:653:TRP:HE1	1:B:688:ASN:HD22	1.37	0.72
1:B:582:GLY:HA2	1:B:616:THR:HB	1.72	0.71
1:A:193:PHE:CD1	1:B:311:THR:HG21	2.26	0.71
1:A:268:LEU:HD13	1:C:193:PHE:CD1	2.25	0.71
1:A:362:ARG:HB3	3:A:1743:N8E:H042	1.73	0.71
1:C:434:LEU:HD21	1:C:522:ILE:HD11	1.72	0.71
1:A:434:LEU:HD21	1:A:522:ILE:HD11	1.73	0.70
1:B:177:LEU:O	1:B:741:LYS:HE3	1.90	0.70
1:B:471:HIS:CE1	1:B:523:ILE:H	2.09	0.70
1:A:304:ARG:HB2	1:A:304:ARG:HH11	1.56	0.70
1:B:396:ASN:HD21	1:B:434:LEU:CG	2.04	0.70
1:A:92:GLU:HG3	4:A:2030:HOH:O	1.90	0.69
1:A:566:PRO:HB2	1:A:576:ARG:HB3	1.75	0.69
1:B:156:ALA:HB3	1:B:447:GLU:HG3	1.75	0.69
1:B:396:ASN:ND2	1:B:434:LEU:HD12	2.08	0.68
1:A:423:ARG:HH11	1:A:423:ARG:CG	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:ARG:HG2	1:B:601:THR:HG22	1.74	0.68
1:C:271:MET:HE3	4:C:2038:HOH:O	1.93	0.68
1:C:403:THR:O	1:C:415:PRO:O	2.11	0.68
1:A:116:SER:HB2	1:A:164:ASN:HB2	1.76	0.68
1:B:65:SER:O	1:B:151:LYS:HE3	1.94	0.67
1:A:285:PHE:CG	1:A:294:ILE:HD11	2.29	0.67
1:B:253:ALA:CB	3:B:1743:N8E:H062	2.25	0.67
1:A:336:GLU:HG3	1:A:358:ARG:HG2	1.76	0.66
1:B:270:HIS:HD2	3:B:1743:N8E:H052	1.61	0.66
1:A:209:GLU:OE1	1:C:740:TYR:OH	2.13	0.66
1:B:81:THR:CG2	1:B:735:ARG:HD3	2.25	0.66
1:C:156:ALA:HB3	1:C:447:GLU:HG3	1.78	0.66
1:C:234:ASN:O	1:C:235:VAL:HB	1.94	0.66
1:B:649:LEU:HD13	1:B:694:TRP:HB3	1.78	0.66
1:A:81:THR:HG22	4:A:2015:HOH:O	1.94	0.65
1:B:116:SER:HB2	1:B:164:ASN:HB2	1.79	0.65
1:B:336:GLU:OE1	1:B:356:HIS:CE1	2.49	0.65
1:A:66:LYS:HD2	1:A:538:GLU:CD	2.22	0.65
1:B:396:ASN:ND2	1:B:434:LEU:CD1	2.60	0.64
1:B:573:VAL:HG22	1:B:576:ARG:HE	1.62	0.64
1:C:434:LEU:HD21	1:C:522:ILE:CD1	2.26	0.64
1:A:219:ASN:HB3	4:A:2068:HOH:O	1.97	0.64
1:B:193:PHE:CD1	1:C:311:THR:HG21	2.33	0.64
1:A:434:LEU:HD21	1:A:522:ILE:CD1	2.28	0.64
1:B:77:LYS:HE3	4:B:2033:HOH:O	1.98	0.64
1:C:73:THR:HG23	1:C:76:GLN:H	1.63	0.64
1:C:164:ASN:ND2	1:C:557:GLN:HE21	1.95	0.64
1:B:682:ARG:NH2	1:B:721:GLN:O	2.31	0.64
1:B:64:GLY:H	1:B:542:ASN:HD21	1.46	0.63
1:C:612:ARG:NH1	1:C:631:GLN:HE21	1.96	0.63
1:C:234:ASN:O	1:C:235:VAL:CB	2.47	0.63
1:C:682:ARG:HD2	4:C:2107:HOH:O	1.97	0.63
1:A:164:ASN:ND2	1:A:557:GLN:HE21	1.97	0.63
1:A:191:SER:HB2	3:B:1743:N8E:H082	1.81	0.63
1:C:153:ALA:HA	1:C:162:ALA:O	1.99	0.63
1:A:145:LYS:HD2	1:A:176:ASP:OD2	1.99	0.63
1:A:612:ARG:HH12	1:A:631:GLN:HE21	1.47	0.63
1:C:672:ASP:O	1:C:674:LYS:N	2.33	0.62
1:B:164:ASN:ND2	1:B:557:GLN:HE21	1.97	0.62
1:A:401:ILE:O	1:A:423:ARG:NH2	2.32	0.62
1:A:304:ARG:HE	1:A:337:ARG:HH21	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ARG:HD2	4:B:2052:HOH:O	1.99	0.62
1:B:434:LEU:HD21	1:B:522:ILE:CD1	2.30	0.62
1:B:736:LEU:HD21	1:C:268:LEU:HD11	1.82	0.62
1:A:268:LEU:HD13	1:C:193:PHE:CE1	2.34	0.61
1:C:251:TYR:HE1	1:C:272:LYS:HD2	1.65	0.61
1:B:566:PRO:HG2	1:B:576:ARG:HD2	1.82	0.61
1:A:172:VAL:O	1:A:254:LYS:HE2	2.01	0.61
1:B:492:HIS:CD2	1:B:494:HIS:H	2.19	0.61
1:A:329:ASN:HD22	1:A:365:ASN:HD22	1.49	0.61
1:B:434:LEU:HD21	1:B:522:ILE:HD11	1.83	0.60
1:B:92:GLU:HG3	4:B:2011:HOH:O	2.00	0.60
1:B:536:ASN:HB2	1:B:557:GLN:OE1	2.01	0.60
1:B:482:ASN:ND2	1:B:533:ARG:HE	2.00	0.60
1:C:73:THR:CG2	1:C:76:GLN:HG3	2.32	0.60
1:A:247:ASP:HB3	1:A:276:ARG:HG2	1.83	0.60
1:A:81:THR:HG21	1:A:707:SER:OG	2.01	0.60
1:C:121:VAL:HG21	1:C:271:MET:CE	2.32	0.60
1:A:121:VAL:HG21	1:A:271:MET:HE1	1.83	0.59
1:B:567:GLN:CD	1:B:579:VAL:HG11	2.27	0.59
1:C:64:GLY:N	1:C:542:ASN:HD21	1.97	0.59
1:A:304:ARG:HH11	1:A:304:ARG:CB	2.14	0.59
1:B:270:HIS:CD2	3:B:1743:N8E:H052	2.37	0.59
1:A:703:ASN:HD22	1:A:739:ASN:HD21	1.47	0.59
1:A:471:HIS:HD2	1:A:516:THR:O	1.86	0.59
1:B:293:ARG:HD2	1:B:673:ARG:NE	2.18	0.59
1:A:177:LEU:O	1:A:741:LYS:HE3	2.03	0.59
1:A:492:HIS:CD2	1:A:494:HIS:H	2.19	0.59
1:A:482:ASN:ND2	1:A:533:ARG:HE	2.01	0.59
1:C:466:PHE:O	1:C:477:SER:HB3	2.03	0.59
1:C:77:LYS:NZ	1:C:144:VAL:O	2.36	0.59
1:C:662:THR:O	1:C:680:VAL:O	2.20	0.59
1:A:156:ALA:HB3	1:A:447:GLU:HG3	1.84	0.58
1:A:582:GLY:HA2	1:A:616:THR:HB	1.85	0.58
1:B:419:GLN:O	1:B:420:MET:C	2.44	0.58
1:A:492:HIS:HD2	1:A:494:HIS:H	1.52	0.58
1:B:419:GLN:O	1:B:422:ASP:N	2.36	0.58
1:A:304:ARG:HH11	1:A:304:ARG:CG	2.16	0.58
1:A:536:ASN:HB2	1:A:557:GLN:OE1	2.04	0.57
1:A:120:LYS:HG2	1:A:125:TYR:CD1	2.40	0.57
1:B:91:GLU:OE2	1:B:639:SER:HB3	2.04	0.57
1:B:425:ASP:OD2	1:B:572:SER:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:702:LEU:HD13	1:C:740:TYR:HB2	1.85	0.57
1:A:304:ARG:HE	1:A:337:ARG:NH2	2.02	0.57
1:B:471:HIS:HD2	1:B:516:THR:O	1.88	0.57
1:A:77:LYS:NZ	1:A:144:VAL:O	2.38	0.57
1:A:112:MET:HE2	1:A:164:ASN:OD1	2.04	0.57
1:B:193:PHE:CE1	1:C:311:THR:HG21	2.40	0.57
1:A:373:ALA:HB3	1:A:376:THR:HG23	1.86	0.57
1:B:336:GLU:OE1	1:B:356:HIS:HE1	1.85	0.57
1:A:270:HIS:HB2	1:C:199:VAL:HG21	1.87	0.57
1:C:373:ALA:HB3	1:C:376:THR:HG23	1.87	0.56
1:A:234:ASN:O	1:A:235:VAL:CB	2.53	0.56
1:B:329:ASN:HD22	1:B:365:ASN:HD22	1.54	0.56
1:C:281:VAL:O	1:C:282:ARG:CB	2.45	0.56
1:B:492:HIS:HD2	1:B:494:HIS:H	1.53	0.56
1:C:81:THR:HG23	1:C:735:ARG:HD3	1.87	0.56
1:A:740:TYR:CD2	3:B:1743:N8E:H202	2.40	0.56
1:C:145:LYS:HD2	1:C:176:ASP:OD2	2.06	0.56
1:A:110:ARG:HD3	1:A:555:PHE:CZ	2.41	0.56
1:B:234:ASN:O	1:B:235:VAL:CB	2.53	0.56
1:A:234:ASN:O	1:A:235:VAL:HB	2.05	0.56
1:A:612:ARG:HH12	1:A:631:GLN:NE2	2.03	0.56
1:C:492:HIS:CD2	1:C:494:HIS:H	2.23	0.56
1:A:657:TYR:CE1	1:A:686:GLY:HA3	2.40	0.55
1:C:195:SER:HB3	1:C:734:VAL:HG13	1.87	0.55
1:C:503:TYR:CZ	1:C:535:ARG:HG3	2.41	0.55
1:B:503:TYR:CZ	1:B:535:ARG:HG3	2.41	0.55
1:C:471:HIS:HD2	1:C:516:THR:O	1.88	0.55
1:C:164:ASN:HD21	1:C:557:GLN:HE21	1.53	0.55
1:C:251:TYR:HD1	1:C:272:LYS:HB3	1.72	0.55
3:A:1743:N8E:H162	1:C:734:VAL:HG22	1.89	0.55
1:C:128:SER:OG	1:C:387:GLN:NE2	2.39	0.55
1:A:654:ARG:HD2	4:A:2122:HOH:O	2.06	0.54
1:C:650:GLU:O	1:C:692:ALA:HA	2.07	0.54
1:B:153:ALA:HB3	1:B:536:ASN:HB3	1.89	0.54
1:B:77:LYS:NZ	1:B:144:VAL:O	2.40	0.54
1:C:566:PRO:HB2	1:C:576:ARG:HB3	1.90	0.54
1:A:209:GLU:OE1	1:C:740:TYR:HE1	1.79	0.54
1:A:362:ARG:HG2	1:A:362:ARG:HH11	1.73	0.54
1:C:362:ARG:HG2	1:C:362:ARG:HH11	1.73	0.54
1:B:654:ARG:HD2	4:B:2077:HOH:O	2.08	0.54
1:A:503:TYR:CZ	1:A:535:ARG:HG3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:VAL:HG21	1:C:271:MET:HE2	1.90	0.54
1:B:241:VAL:CG1	1:B:286:THR:HG21	2.38	0.54
1:A:613:PHE:CD1	1:A:613:PHE:N	2.75	0.53
1:A:736:LEU:HD22	1:B:268:LEU:CD1	2.38	0.53
1:C:329:ASN:HD22	1:C:365:ASN:HD22	1.55	0.53
1:B:538:GLU:HB2	1:B:554:TYR:O	2.08	0.53
1:B:672:ASP:OD1	1:B:676:ASN:HB2	2.08	0.53
1:C:392:GLN:HB3	4:C:2082:HOH:O	2.08	0.53
1:A:195:SER:HB3	1:A:734:VAL:HG13	1.90	0.53
1:C:672:ASP:O	1:C:672:ASP:OD1	2.27	0.53
1:B:234:ASN:O	1:B:235:VAL:HG12	2.09	0.53
1:C:529:THR:HA	1:C:580:ASN:HD21	1.73	0.53
1:B:293:ARG:HD2	1:B:673:ARG:CZ	2.37	0.53
1:A:153:ALA:HB3	1:A:536:ASN:HB3	1.91	0.53
1:A:268:LEU:HD22	1:C:193:PHE:CZ	2.42	0.53
1:B:253:ALA:HB3	3:B:1743:N8E:H062	1.91	0.53
1:A:201:TYR:CE1	3:B:1743:N8E:H013	2.39	0.53
1:B:672:ASP:C	1:B:674:LYS:N	2.64	0.53
1:C:184:ASN:ND2	1:C:208:LYS:HE3	2.23	0.53
1:B:234:ASN:O	1:B:235:VAL:HB	2.09	0.53
1:B:530:LYS:H	1:B:580:ASN:HD21	1.58	0.52
1:C:549:ALA:O	1:C:593:ALA:HA	2.09	0.52
1:A:653:TRP:HE1	1:A:688:ASN:HD22	1.55	0.52
1:C:612:ARG:HH22	1:C:631:GLN:HE21	1.57	0.52
1:A:64:GLY:N	1:A:542:ASN:HD21	2.04	0.52
1:A:419:GLN:O	1:A:423:ARG:HD2	2.09	0.52
1:C:633:GLY:HA3	1:C:659:GLN:O	2.10	0.52
1:A:66:LYS:HB2	1:A:538:GLU:OE2	2.09	0.52
1:B:153:ALA:HA	1:B:162:ALA:O	2.10	0.52
1:B:526:ALA:O	1:B:529:THR:CG2	2.58	0.52
1:C:75:GLN:NE2	1:C:700:ASP:OD2	2.43	0.52
1:A:241:VAL:CG1	1:A:286:THR:HG21	2.40	0.51
1:C:65:SER:O	1:C:151:LYS:HE3	2.11	0.51
1:A:153:ALA:HA	1:A:162:ALA:O	2.10	0.51
1:A:304:ARG:HD2	4:A:2082:HOH:O	2.11	0.51
1:C:482:ASN:ND2	1:C:533:ARG:HE	2.09	0.51
1:A:281:VAL:O	1:A:299:GLN:OE1	2.29	0.51
1:A:133:HIS:CG	1:A:282:ARG:HG2	2.46	0.51
1:C:717:TYR:CZ	1:C:725:ASN:HB3	2.46	0.51
1:A:270:HIS:CD2	1:C:199:VAL:HG11	2.46	0.50
1:A:286:THR:O	1:A:294:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ASN:HB2	1:B:627:GLU:HG2	1.93	0.50
1:B:113:GLY:HA3	1:B:627:GLU:O	2.11	0.50
1:A:499:ALA:HA	1:A:538:GLU:O	2.10	0.50
1:B:420:MET:O	1:B:423:ARG:N	2.44	0.50
1:C:672:ASP:O	1:C:672:ASP:CG	2.53	0.50
1:A:606:VAL:HA	1:A:635:THR:O	2.11	0.50
1:A:682:ARG:HD2	4:A:2119:HOH:O	2.11	0.50
1:B:286:THR:HG23	1:B:727:LEU:HD21	1.94	0.50
1:A:359:ILE:HD11	1:A:513:ALA:HB2	1.93	0.50
3:A:1743:N8E:H132	1:C:193:PHE:HB3	1.92	0.50
1:B:373:ALA:HB3	1:B:376:THR:HG23	1.92	0.50
1:A:241:VAL:HG12	1:A:286:THR:HG21	1.94	0.50
1:B:286:THR:HG23	1:B:727:LEU:CD2	2.42	0.50
1:B:93:PRO:HB2	1:B:607:SER:HB3	1.93	0.50
1:B:220:ARG:HG3	1:B:249:ARG:HG2	1.93	0.50
1:C:63:GLN:OE1	1:C:67:ILE:HD12	2.12	0.49
1:C:73:THR:HG22	1:C:76:GLN:CG	2.41	0.49
1:C:247:ASP:HB3	1:C:276:ARG:HG2	1.94	0.49
1:B:437:PRO:HG3	1:B:471:HIS:HB3	1.93	0.49
1:C:71:ILE:HD11	1:C:149:VAL:HG12	1.93	0.49
1:C:81:THR:HG21	1:C:707:SER:OG	2.12	0.49
1:C:422:ASP:O	1:C:425:ASP:N	2.46	0.49
1:B:164:ASN:HD21	1:B:557:GLN:HE21	1.59	0.49
1:C:120:LYS:HG2	1:C:125:TYR:CD1	2.48	0.49
1:C:116:SER:HB2	1:C:164:ASN:HB2	1.94	0.49
1:A:657:TYR:CD1	1:A:686:GLY:HA3	2.46	0.49
1:B:649:LEU:CD1	1:B:694:TRP:HB3	2.43	0.49
1:B:688:ASN:O	1:B:711:VAL:HG23	2.13	0.49
1:C:530:LYS:H	1:C:580:ASN:HD21	1.61	0.49
1:B:108:THR:HG23	1:B:720:SER:HB3	1.95	0.49
1:A:530:LYS:N	1:A:580:ASN:HD21	2.05	0.49
1:B:81:THR:HG21	1:B:707:SER:OG	2.12	0.49
1:B:281:VAL:O	1:B:282:ARG:CB	2.46	0.49
1:A:209:GLU:CD	1:C:740:TYR:OH	2.56	0.49
1:A:234:ASN:O	1:A:235:VAL:HG12	2.13	0.49
1:A:268:LEU:HB3	1:C:193:PHE:CZ	2.47	0.48
1:B:184:ASN:ND2	1:B:208:LYS:HE3	2.28	0.48
1:B:526:ALA:O	1:B:529:THR:HG23	2.14	0.48
1:C:77:LYS:HE2	4:C:2006:HOH:O	2.11	0.48
1:C:658:VAL:HG13	1:C:685:PHE:CE1	2.48	0.48
1:A:73:THR:HG22	1:A:76:GLN:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ARG:CG	1:B:362:ARG:NH1	2.54	0.48
1:C:92:GLU:HG3	4:C:2022:HOH:O	2.12	0.48
1:C:341:ASP:OD1	1:C:343:SER:OG	2.31	0.48
1:A:71:ILE:HD11	1:A:149:VAL:HG12	1.95	0.48
3:A:1743:N8E:H132	1:C:193:PHE:CD2	2.49	0.48
4:A:2074:HOH:O	3:B:1743:N8E:H011	2.14	0.48
1:B:121:VAL:HG21	1:B:271:MET:HE1	1.95	0.48
1:B:736:LEU:HD21	1:C:268:LEU:CD1	2.42	0.48
1:C:197:ASN:HB3	1:C:224:LYS:HB2	1.95	0.48
1:A:195:SER:CB	1:A:734:VAL:HG13	2.44	0.48
1:C:437:PRO:HG3	1:C:471:HIS:HB3	1.96	0.48
1:A:705:ASN:O	1:A:736:LEU:HA	2.14	0.48
1:B:703:ASN:HD22	1:B:739:ASN:ND2	2.05	0.48
1:B:145:LYS:HD2	1:B:176:ASP:OD2	2.13	0.47
1:B:66:LYS:HB2	1:B:538:GLU:OE2	2.15	0.47
1:A:608:HIS:HE1	4:A:2116:HOH:O	1.97	0.47
1:A:623:SER:HB3	1:A:628:PHE:CE2	2.50	0.47
1:A:694:TRP:O	1:A:696:PRO:HD3	2.15	0.47
1:C:723:TRP:C	1:C:724:THR:O	2.54	0.47
1:A:99:GLY:H	1:A:721:GLN:NE2	2.12	0.47
1:A:99:GLY:H	1:A:721:GLN:HE22	1.62	0.47
1:A:191:SER:HB2	3:B:1743:N8E:H102	1.95	0.47
1:B:66:LYS:HD2	1:B:538:GLU:CD	2.39	0.47
1:B:133:HIS:CG	1:B:282:ARG:HG2	2.50	0.47
1:A:286:THR:HG23	1:A:727:LEU:CD2	2.44	0.47
1:B:251:TYR:HD1	1:B:272:LYS:HB3	1.80	0.46
1:C:390:LYS:HG2	1:C:436:ASN:ND2	2.30	0.46
1:B:247:ASP:HB3	1:B:276:ARG:HG2	1.97	0.46
1:A:145:LYS:HB3	1:A:172:VAL:HA	1.98	0.46
1:C:425:ASP:O	1:C:429:VAL:HG23	2.15	0.46
1:C:492:HIS:HD2	1:C:494:HIS:HB2	1.81	0.46
1:C:612:ARG:NH1	1:C:631:GLN:NE2	2.49	0.46
1:A:268:LEU:HD22	1:C:193:PHE:CD2	2.49	0.46
1:A:415:PRO:O	1:A:419:GLN:HG3	2.16	0.46
1:C:492:HIS:HD2	1:C:494:HIS:H	1.63	0.46
1:B:736:LEU:CD2	1:C:268:LEU:CD1	2.83	0.46
1:C:178:LEU:O	1:C:179:LYS:C	2.59	0.46
1:A:110:ARG:HD3	1:A:555:PHE:CE2	2.51	0.46
1:A:613:PHE:N	1:A:613:PHE:HD1	2.15	0.45
1:A:682:ARG:NH2	1:A:721:GLN:O	2.49	0.45
1:B:72:VAL:HG11	1:B:88:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:ASP:OD1	1:B:709:ASN:HA	2.16	0.45
1:A:164:ASN:HD21	1:A:557:GLN:HE21	1.63	0.45
1:B:64:GLY:N	1:B:542:ASN:HD21	2.12	0.45
1:C:632:VAL:HG13	1:C:719:HIS:HB2	1.99	0.45
1:B:121:VAL:HA	1:B:169:ALA:O	2.16	0.45
1:C:420:MET:HE3	1:C:420:MET:HB2	1.81	0.45
1:C:658:VAL:CG1	1:C:685:PHE:CZ	2.99	0.45
1:B:643:ARG:NH2	1:B:693:ASN:OD1	2.46	0.45
1:A:503:TYR:CE2	1:A:535:ARG:HG3	2.52	0.45
1:B:253:ALA:HB2	3:B:1743:N8E:H062	1.98	0.45
1:C:133:HIS:CG	1:C:282:ARG:HG2	2.52	0.45
1:C:499:ALA:HA	1:C:538:GLU:O	2.17	0.45
1:A:113:GLY:HA3	1:A:627:GLU:O	2.17	0.45
1:A:392:GLN:HG3	1:C:243:TYR:OH	2.17	0.45
1:A:466:PHE:O	1:A:477:SER:HB3	2.17	0.45
1:C:536:ASN:HB2	1:C:557:GLN:OE1	2.17	0.45
1:C:703:ASN:HB2	1:C:739:ASN:ND2	2.32	0.45
1:A:181:LEU:HD21	1:A:741:LYS:HB3	1.98	0.45
1:A:616:THR:HG21	4:A:2112:HOH:O	2.17	0.45
1:B:489:TRP:CE2	1:B:491:PRO:HG3	2.52	0.45
1:B:312:ASN:OD1	1:B:329:ASN:OD1	2.34	0.45
1:C:526:ALA:O	1:C:529:THR:CG2	2.65	0.44
1:A:426:GLU:H	1:A:426:GLU:HG2	1.47	0.44
1:B:251:TYR:CD1	3:B:1743:N8E:H031	2.52	0.44
1:B:335:LYS:HD2	4:B:2030:HOH:O	2.18	0.44
1:B:499:ALA:HA	1:B:538:GLU:O	2.16	0.44
1:A:305:GLU:OE1	2:A:1744:GLU:HB2	2.18	0.44
1:A:545:ASP:OD1	1:A:545:ASP:C	2.60	0.44
1:A:270:HIS:CB	1:C:199:VAL:HG21	2.47	0.44
1:B:658:VAL:O	1:B:684:GLY:HA2	2.18	0.44
1:A:416:MET:SD	1:A:419:GLN:NE2	2.91	0.44
1:C:492:HIS:HB3	1:C:495:TRP:HD1	1.83	0.44
1:A:736:LEU:HD22	1:B:268:LEU:HD12	1.99	0.44
1:C:332:VAL:HG13	1:C:332:VAL:O	2.18	0.44
1:A:533:ARG:HD3	4:A:2106:HOH:O	2.17	0.44
1:A:610:LYS:HA	1:A:631:GLN:HE22	1.83	0.44
1:B:335:LYS:HE2	1:B:335:LYS:HB2	1.36	0.44
1:C:564:ALA:HB3	1:C:622:LEU:HA	2.00	0.44
1:A:507:SER:O	1:A:509:ARG:NH1	2.51	0.43
1:C:658:VAL:HG13	1:C:685:PHE:CZ	2.53	0.43
1:A:341:ASP:OD1	1:A:343:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:LYS:O	1:C:422:ASP:C	2.60	0.43
1:C:623:SER:HB3	1:C:628:PHE:CE2	2.53	0.43
1:B:195:SER:HB3	1:B:734:VAL:HG13	1.98	0.43
1:A:143:LEU:HD13	1:A:271:MET:SD	2.58	0.43
1:C:730:VAL:HG12	1:C:731:GLY:O	2.18	0.43
1:B:145:LYS:HG2	1:B:146:VAL:HG22	1.99	0.43
1:C:489:TRP:CE2	1:C:491:PRO:HG3	2.53	0.43
1:C:730:VAL:HG23	4:C:2017:HOH:O	2.17	0.43
1:A:285:PHE:CG	1:A:294:ILE:CD1	3.01	0.43
1:A:559:ILE:HB	1:A:584:ILE:HB	2.00	0.43
1:A:703:ASN:HB2	1:A:739:ASN:ND2	2.33	0.43
1:A:437:PRO:HG3	1:A:471:HIS:HB3	2.01	0.43
1:B:110:ARG:HD3	1:B:555:PHE:CZ	2.54	0.43
1:C:151:LYS:NZ	1:C:590:GLU:OE1	2.47	0.43
1:C:549:ALA:HB3	1:C:594:SER:OG	2.18	0.43
1:B:329:ASN:HB2	4:B:2023:HOH:O	2.18	0.43
1:A:362:ARG:HG2	1:A:362:ARG:NH1	2.33	0.43
1:A:526:ALA:O	1:A:529:THR:HG23	2.19	0.43
1:A:133:HIS:CD2	1:A:282:ARG:HG2	2.54	0.43
1:A:368:PHE:CD1	1:A:368:PHE:N	2.86	0.43
1:B:323:VAL:HG21	1:B:368:PHE:HB3	2.01	0.43
1:B:726:THR:OG1	1:B:727:LEU:N	2.51	0.43
1:C:503:TYR:CE2	1:C:535:ARG:HG3	2.54	0.43
1:A:333:LEU:HB3	1:A:361:THR:HB	2.00	0.42
1:B:241:VAL:HG13	1:B:286:THR:HG21	1.99	0.42
1:B:623:SER:HB3	1:B:628:PHE:CE2	2.55	0.42
1:C:541:PHE:O	1:C:551:ASN:HA	2.19	0.42
1:C:653:TRP:NE1	1:C:688:ASN:HD22	2.00	0.42
1:C:736:LEU:HG	1:C:737:GLY:N	2.34	0.42
1:B:286:THR:O	1:B:294:ILE:HG12	2.20	0.42
1:B:369:ASP:HB3	1:B:377:LEU:HD11	2.01	0.42
1:C:251:TYR:CD1	1:C:272:LYS:HB3	2.53	0.42
1:C:259:PHE:HE1	1:C:266:ILE:HD12	1.83	0.42
1:A:193:PHE:CE1	1:B:311:THR:CG2	2.88	0.42
1:B:294:ILE:HG21	1:B:294:ILE:HD13	1.79	0.42
1:C:133:HIS:CD2	1:C:282:ARG:HG2	2.55	0.42
1:C:286:THR:O	1:C:294:ILE:HG12	2.19	0.42
1:C:618:LYS:HE2	1:C:618:LYS:H	1.84	0.42
1:B:234:ASN:O	1:B:235:VAL:CG1	2.67	0.42
1:C:538:GLU:HB2	1:C:554:TYR:O	2.19	0.42
1:A:281:VAL:O	1:A:282:ARG:CB	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASP:O	1:A:425:ASP:HB2	2.20	0.42
1:A:725:ASN:HD22	1:A:725:ASN:HA	1.72	0.42
1:B:128:SER:OG	1:B:387:GLN:NE2	2.53	0.42
1:B:133:HIS:CD2	1:B:282:ARG:HG2	2.55	0.42
1:C:71:ILE:HD11	1:C:149:VAL:CG1	2.50	0.42
1:A:71:ILE:HD11	1:A:149:VAL:CG1	2.49	0.42
1:A:311:THR:HG23	1:C:193:PHE:HE2	1.84	0.42
1:A:375:GLN:CA	1:A:375:GLN:OE1	2.68	0.42
1:B:91:GLU:CD	1:B:639:SER:HB3	2.44	0.42
1:B:241:VAL:HG12	1:B:286:THR:HG21	2.01	0.42
1:A:454:ASP:HB2	1:A:490:GLN:O	2.19	0.42
1:A:67:ILE:HD11	4:A:2004:HOH:O	2.19	0.42
1:A:93:PRO:HB2	1:A:607:SER:HB3	2.02	0.42
1:A:251:TYR:OH	1:A:272:LYS:HE3	2.20	0.42
1:C:612:ARG:NH2	1:C:631:GLN:HE21	2.17	0.42
1:B:258:THR:OG1	1:B:265:ARG:NH1	2.50	0.42
1:B:650:GLU:O	1:B:692:ALA:HA	2.20	0.42
1:C:289:ASP:OD2	1:C:291:SER:OG	2.30	0.42
1:C:715:PHE:HA	4:C:2071:HOH:O	2.19	0.41
1:A:723:TRP:C	1:A:724:THR:O	2.61	0.41
1:B:396:ASN:HD21	1:B:434:LEU:CD1	2.24	0.41
1:C:139:VAL:HG23	4:C:2076:HOH:O	2.18	0.41
1:A:526:ALA:O	1:A:529:THR:CG2	2.68	0.41
1:B:143:LEU:HD13	1:B:271:MET:SD	2.60	0.41
1:B:507:SER:O	1:B:509:ARG:NH1	2.54	0.41
1:A:532:GLU:HG3	1:A:563:LEU:HD12	2.03	0.41
1:B:282:ARG:HA	4:B:2028:HOH:O	2.19	0.41
1:C:172:VAL:O	1:C:254:LYS:HE2	2.19	0.41
1:A:678:GLU:CD	1:A:723:TRP:HE1	2.29	0.41
1:B:251:TYR:CD1	1:B:272:LYS:HB3	2.55	0.41
1:B:545:ASP:C	1:B:545:ASP:OD1	2.63	0.41
1:A:73:THR:HG22	1:A:75:GLN:N	2.35	0.41
1:B:569:ARG:HD2	1:B:577:GLU:OE2	2.21	0.41
1:B:703:ASN:HB2	1:B:739:ASN:ND2	2.36	0.41
1:A:121:VAL:HA	1:A:169:ALA:O	2.21	0.41
1:A:649:LEU:CD1	1:A:694:TRP:HB3	2.50	0.41
1:A:270:HIS:CG	1:C:199:VAL:HG11	2.56	0.41
1:A:311:THR:CG2	1:C:193:PHE:HE2	2.34	0.41
1:A:613:PHE:HB2	1:A:666:LEU:HD23	2.02	0.41
1:C:171:THR:OG1	1:C:254:LYS:NZ	2.51	0.41
1:C:294:ILE:HG21	1:C:294:ILE:HD13	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:MET:O	1:C:423:ARG:HB2	2.20	0.41
1:C:541:PHE:CD1	1:C:541:PHE:C	2.99	0.41
1:C:545:ASP:OD1	1:C:545:ASP:C	2.64	0.41
1:A:81:THR:CG2	1:A:735:ARG:HD3	2.44	0.41
1:B:567:GLN:HB3	1:B:579:VAL:HG21	2.03	0.41
1:C:616:THR:HG21	4:C:2099:HOH:O	2.20	0.41
1:A:158:ALA:HB2	4:A:2062:HOH:O	2.20	0.40
1:B:395:LEU:O	1:B:398:LYS:HB2	2.21	0.40
1:C:188:ARG:HG3	1:C:741:LYS:HG3	2.03	0.40
1:B:482:ASN:HA	1:B:483:PRO:HD3	1.92	0.40
1:B:672:ASP:O	1:B:672:ASP:CG	2.65	0.40
1:A:529:THR:HA	1:A:580:ASN:ND2	2.36	0.40
1:A:619:ASP:O	1:A:621:LEU:HG	2.22	0.40
1:C:375:GLN:OE1	1:C:375:GLN:N	2.54	0.40
1:C:97:PHE:CE2	1:C:107:LEU:HD12	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	653/742 (88%)	626 (96%)	23 (4%)	4 (1%)	21	32
1	B	659/742 (89%)	629 (95%)	24 (4%)	6 (1%)	14	22
1	C	659/742 (89%)	623 (94%)	30 (5%)	6 (1%)	14	22
All	All	1971/2226 (88%)	1878 (95%)	77 (4%)	16 (1%)	16	25

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	VAL
1	A	396	ASN

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Mol	Chain	Res	Type
1	A	724	THR
1	B	235	VAL
1	B	396	ASN
1	C	235	VAL
1	C	396	ASN
1	C	420	MET
1	A	511	TYR
1	B	620	LYS
1	B	673	ARG
1	C	598	GLY
1	C	422	ASP
1	C	724	THR
1	B	421	LYS
1	B	64	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	542/612 (89%)	479 (88%)	63 (12%)	5	8
1	B	544/612 (89%)	481 (88%)	63 (12%)	5	8
1	C	546/612 (89%)	487 (89%)	59 (11%)	6	9
All	All	1632/1836 (89%)	1447 (89%)	185 (11%)	5	8

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	73	THR
1	A	75	GLN
1	A	81	THR
1	A	116	SER
1	A	117	VAL
1	A	121	VAL
1	A	145	LYS

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Mol	Chain	Res	Type
1	A	150	GLN
1	A	164	ASN
1	A	173	ASP
1	A	199	VAL
1	A	212	PHE
1	A	224	LYS
1	A	235	VAL
1	A	255	ILE
1	A	272	LYS
1	A	276	ARG
1	A	290	LYS
1	A	304	ARG
1	A	306	THR
1	A	316	THR
1	A	320	LEU
1	A	324	GLU
1	A	327	ASP
1	A	333	LEU
1	A	335	LYS
1	A	343	SER
1	A	356	HIS
1	A	367	ASN
1	A	370	SER
1	A	376	THR
1	A	382	ILE
1	A	417	GLU
1	A	423	ARG
1	A	426	GLU
1	A	435	SER
1	A	442	THR
1	A	446	ILE
1	A	447	GLU
1	A	452	ILE
1	A	461	LEU
1	A	465	ARG
1	A	471	HIS
1	A	475	THR
1	A	477	SER
1	A	529	THR
1	A	585	LYS
1	A	601	THR
1	A	604	VAL

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Mol	Chain	Res	Type
1	A	613	PHE
1	A	616	THR
1	A	634	ARG
1	A	643	ARG
1	A	658	VAL
1	A	662	THR
1	A	676	ASN
1	A	694	TRP
1	A	714	LYS
1	A	732	ARG
1	A	734	VAL
1	A	736	LEU
1	A	739	ASN
1	B	75	GLN
1	B	81	THR
1	B	95	ILE
1	B	116	SER
1	B	117	VAL
1	B	121	VAL
1	B	144	VAL
1	B	150	GLN
1	B	173	ASP
1	B	199	VAL
1	B	235	VAL
1	B	251	TYR
1	B	255	ILE
1	B	268	LEU
1	B	276	ARG
1	B	290	LYS
1	B	306	THR
1	B	309	SER
1	B	316	THR
1	B	323	VAL
1	B	333	LEU
1	B	335	LYS
1	B	343	SER
1	B	362	ARG
1	B	370	SER
1	B	376	THR
1	B	382	ILE
1	B	397	SER
1	B	400	SER

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Mol	Chain	Res	Type
1	B	417	GLU
1	B	419	GLN
1	B	428	THR
1	B	435	SER
1	B	442	THR
1	B	446	ILE
1	B	447	GLU
1	B	452	ILE
1	B	461	LEU
1	B	465	ARG
1	B	471	HIS
1	B	475	THR
1	B	477	SER
1	B	507	SER
1	B	529	THR
1	B	572	SER
1	B	575	VAL
1	B	579	VAL
1	B	585	LYS
1	B	604	VAL
1	B	616	THR
1	B	623	SER
1	B	634	ARG
1	B	643	ARG
1	B	645	GLN
1	B	651	ILE
1	B	658	VAL
1	B	677	LEU
1	B	682	ARG
1	B	694	TRP
1	B	699	LYS
1	B	714	LYS
1	B	739	ASN
1	B	741	LYS
1	C	75	GLN
1	C	81	THR
1	C	116	SER
1	C	117	VAL
1	C	121	VAL
1	C	144	VAL
1	C	146	VAL
1	C	173	ASP

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Mol	Chain	Res	Type
1	C	199	VAL
1	C	224	LYS
1	C	235	VAL
1	C	251	TYR
1	C	255	ILE
1	C	266	ILE
1	C	268	LEU
1	C	276	ARG
1	C	286	THR
1	C	290	LYS
1	C	309	SER
1	C	316	THR
1	C	333	LEU
1	C	335	LYS
1	C	343	SER
1	C	370	SER
1	C	376	THR
1	C	382	ILE
1	C	403	THR
1	C	420	MET
1	C	435	SER
1	C	442	THR
1	C	446	ILE
1	C	447	GLU
1	C	452	ILE
1	C	461	LEU
1	C	465	ARG
1	C	471	HIS
1	C	475	THR
1	C	477	SER
1	C	481	LEU
1	C	529	THR
1	C	530	LYS
1	C	563	LEU
1	C	575	VAL
1	C	579	VAL
1	C	585	LYS
1	C	604	VAL
1	C	616	THR
1	C	618	LYS
1	C	643	ARG
1	C	645	GLN

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Mol	Chain	Res	Type
1	C	658	VAL
1	C	662	THR
1	C	677	LEU
1	C	694	TRP
1	C	697	LEU
1	C	714	LYS
1	C	732	ARG
1	C	734	VAL
1	C	739	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	164	ASN
1	A	184	ASN
1	A	264	HIS
1	A	329	ASN
1	A	387	GLN
1	A	419	GLN
1	A	471	HIS
1	A	482	ASN
1	A	492	HIS
1	A	494	HIS
1	A	542	ASN
1	A	567	GLN
1	A	580	ASN
1	A	608	HIS
1	A	631	GLN
1	A	688	ASN
1	A	721	GLN
1	A	725	ASN
1	A	739	ASN
1	B	150	GLN
1	B	164	ASN
1	B	175	GLN
1	B	184	ASN
1	B	274	GLN
1	B	329	ASN
1	B	356	HIS
1	B	387	GLN
1	B	396	ASN

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Mol	Chain	Res	Type
1	B	436	ASN
1	B	471	HIS
1	B	482	ASN
1	B	492	HIS
1	B	494	HIS
1	B	542	ASN
1	B	580	ASN
1	B	670	GLN
1	B	688	ASN
1	B	709	ASN
1	B	739	ASN
1	C	75	GLN
1	C	164	ASN
1	C	184	ASN
1	C	274	GLN
1	C	329	ASN
1	C	387	GLN
1	C	436	ASN
1	C	471	HIS
1	C	482	ASN
1	C	492	HIS
1	C	542	ASN
1	C	580	ASN
1	C	631	GLN
1	C	645	GLN
1	C	670	GLN
1	C	688	ASN
1	C	725	ASN
1	C	739	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	N8E	A	1743	-	23,23,23	0.91	0	22,22,22	1.01	0
3	N8E	B	1743	-	23,23,23	0.46	0	22,22,22	0.68	0
2	GLU	A	1744	-	8,9,9	1.42	2 (25%)	8,11,11	1.55	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	N8E	A	1743	-	-	11/21/21/21	-
3	N8E	B	1743	-	-	13/21/21/21	-
2	GLU	A	1744	-	-	2/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1744	GLU	OXT-C	-2.62	1.22	1.30
2	A	1744	GLU	OE2-CD	-2.02	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1744	GLU	OXT-C-O	-2.79	117.75	124.08
2	A	1744	GLU	CB-CA-C	2.19	116.25	110.45

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1743	N8E	O09-C10-C11-O12
3	B	1743	N8E	O12-C13-C14-O15
3	B	1743	N8E	O18-C19-C20-O21
3	A	1743	N8E	O18-C19-C20-O21
3	A	1743	N8E	C06-C07-C08-O09
3	A	1743	N8E	O15-C16-C17-O18
3	A	1743	N8E	O21-C22-C23-O24
3	A	1743	N8E	C04-C05-C06-C07
3	B	1743	N8E	C02-C03-C04-C05
3	A	1743	N8E	C01-C02-C03-C04
3	B	1743	N8E	C23-C22-O21-C20
3	A	1743	N8E	C02-C03-C04-C05
3	B	1743	N8E	C04-C05-C06-C07
3	A	1743	N8E	C20-C19-O18-C17
3	B	1743	N8E	C03-C04-C05-C06
3	B	1743	N8E	C13-C14-O15-C16
3	B	1743	N8E	C16-C17-O18-C19
3	A	1743	N8E	C13-C14-O15-C16
3	B	1743	N8E	C01-C02-C03-C04
3	A	1743	N8E	C11-C10-O09-C08
3	B	1743	N8E	C19-C20-O21-C22
3	B	1743	N8E	C05-C06-C07-C08
3	B	1743	N8E	C10-C11-O12-C13
3	A	1743	N8E	C16-C17-O18-C19
2	A	1744	GLU	N-CA-CB-CG
2	A	1744	GLU	CA-CB-CG-CD

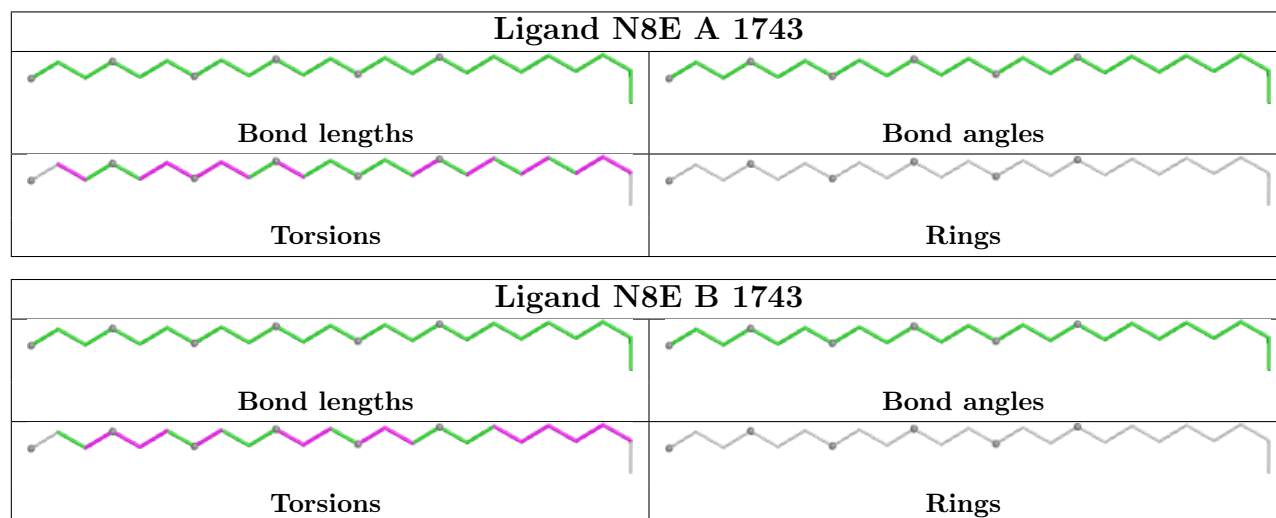
There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1743	N8E	4	0
3	B	1743	N8E	14	0
2	A	1744	GLU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	661/742 (89%)	0.22	40 (6%) 27 23	5, 20, 41, 60	0
1	B	665/742 (89%)	0.21	29 (4%) 39 34	6, 22, 47, 62	0
1	C	665/742 (89%)	0.26	42 (6%) 26 22	5, 20, 46, 62	0
All	All	1991/2226 (89%)	0.23	111 (5%) 30 26	5, 20, 45, 62	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	415	PRO	4.6
1	A	212	PHE	4.1
1	B	193	PHE	4.0
1	A	233	ARG	4.0
1	B	677	LEU	4.0
1	C	416	MET	3.8
1	A	289	ASP	3.8
1	C	372	LEU	3.8
1	A	286	THR	3.7
1	C	322	PHE	3.5
1	B	572	SER	3.3
1	C	193	PHE	3.3
1	C	373	ALA	3.3
1	A	193	PHE	3.2
1	B	417	GLU	3.2
1	C	263	ASP	3.2
1	C	236	ASN	3.2
1	A	237	GLY	3.2
1	B	237	GLY	3.1
1	A	373	ALA	3.1
1	A	180	GLY	3.1
1	B	372	LEU	3.1
1	B	262	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	294	ILE	3.0
1	C	261	ASP	3.0
1	B	294	ILE	3.0
1	C	233	ARG	2.9
1	B	229	GLY	2.9
1	B	230	LYS	2.8
1	B	239	LYS	2.8
1	C	286	THR	2.8
1	A	181	LEU	2.8
1	A	294	ILE	2.8
1	C	546	GLY	2.8
1	C	180	GLY	2.7
1	C	287	VAL	2.7
1	A	231	GLY	2.7
1	C	288	GLY	2.7
1	C	262	ASP	2.7
1	C	344	GLY	2.7
1	A	403	THR	2.7
1	A	208	LYS	2.6
1	A	293	ARG	2.6
1	C	281	VAL	2.6
1	A	297	ASP	2.6
1	A	528	GLY	2.6
1	A	619	ASP	2.6
1	C	259	PHE	2.6
1	C	251	TYR	2.5
1	C	231	GLY	2.5
1	C	237	GLY	2.5
1	A	356	HIS	2.5
1	C	492	HIS	2.5
1	C	547	THR	2.5
1	B	180	GLY	2.5
1	A	281	VAL	2.5
1	C	374	GLU	2.5
1	C	375	GLN	2.5
1	C	485	PHE	2.5
1	B	291	SER	2.5
1	C	182	ASP	2.4
1	B	573	VAL	2.4
1	C	184	ASN	2.4
1	A	209	GLU	2.4
1	A	374	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	231	GLY	2.4
1	B	289	ASP	2.4
1	A	566	PRO	2.4
1	A	210	GLY	2.4
1	C	293	ARG	2.4
1	B	236	ASN	2.4
1	C	402	PRO	2.3
1	A	238	GLY	2.3
1	B	233	ARG	2.3
1	B	182	ASP	2.3
1	C	645	GLN	2.3
1	A	262	ASP	2.3
1	C	239	LYS	2.3
1	A	310	ASN	2.2
1	C	347	TYR	2.3
1	A	261	ASP	2.2
1	B	235	VAL	2.2
1	A	251	TYR	2.2
1	A	290	LYS	2.2
1	B	400	SER	2.2
1	A	182	ASP	2.2
1	A	184	ASN	2.2
1	B	373	ALA	2.2
1	C	421	LYS	2.2
1	A	229	GLY	2.1
1	C	528	GLY	2.1
1	B	290	LYS	2.1
1	B	694	TRP	2.1
1	A	372	LEU	2.1
1	B	286	THR	2.1
1	B	263	ASP	2.1
1	A	230	LYS	2.1
1	A	620	LYS	2.1
1	A	175	GLN	2.1
1	B	674	LYS	2.1
1	C	367	ASN	2.1
1	C	230	LYS	2.1
1	B	232	PHE	2.0
1	A	71	ILE	2.0
1	C	404	THR	2.0
1	A	68	ARG	2.0
1	A	287	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	238	GLY	2.0
1	A	547	THR	2.0
1	C	527	ASP	2.0
1	B	498	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

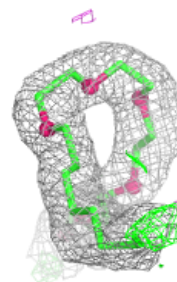
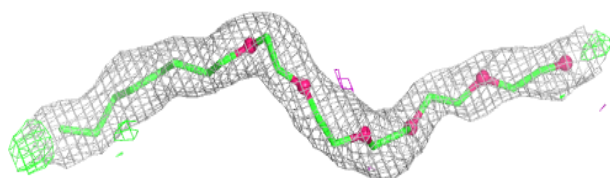
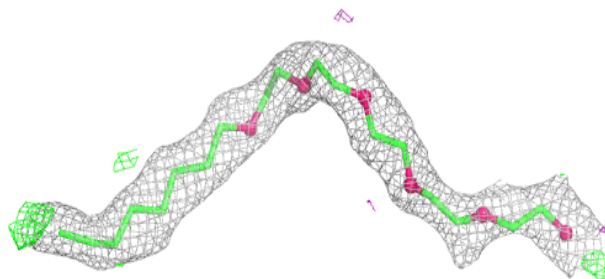
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLU	A	1744	10/10	0.86	0.13	15,20,22,22	0
3	N8E	A	1743	24/24	0.89	0.12	12,19,38,40	0
3	N8E	B	1743	24/24	0.93	0.10	12,20,35,38	0

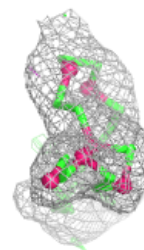
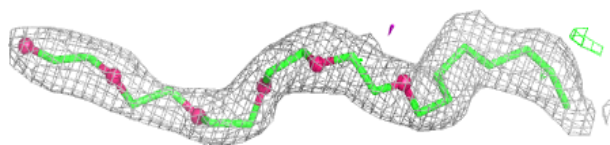
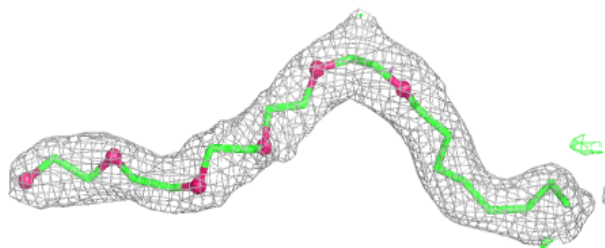
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around N8E A 1743:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around N8E B 1743:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.