



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:57 PM UTC

PDB ID : 6ED1 / pdb_00006ed1
Title : Bacteroides dorei Beta-glucuronidase
Authors : Biernat, K.A.; Redinbo, M.R.
Deposited on : 2018-08-08
Resolution : 2.90 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

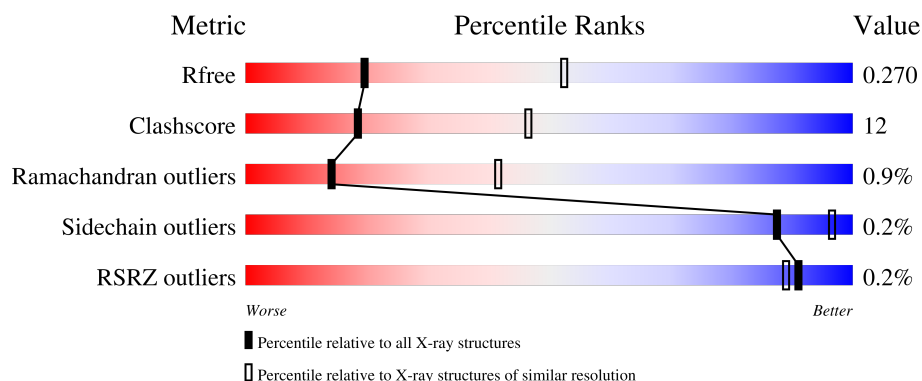
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	879	 70% 27% .
1	B	879	 71% 26% .
1	C	879	 72% 25% ..
1	D	879	 65% 33% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27956 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 Glycosyl hydrolase family 2, sugar binding domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	860	Total	C	N	O	S	0	0	0
			6901	4411	1179	1281	30			
1	B	860	Total	C	N	O	S	0	0	0
			6914	4416	1181	1287	30			
1	C	860	Total	C	N	O	S	0	0	0
			6909	4413	1178	1289	29			
1	D	860	Total	C	N	O	S	0	0	0
			6857	4382	1167	1279	29			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP C3R9X4
A	2	HIS	-	expression tag	UNP C3R9X4
A	3	HIS	-	expression tag	UNP C3R9X4
A	4	HIS	-	expression tag	UNP C3R9X4
A	5	HIS	-	expression tag	UNP C3R9X4
A	6	HIS	-	expression tag	UNP C3R9X4
A	7	HIS	-	expression tag	UNP C3R9X4
A	8	SER	-	expression tag	UNP C3R9X4
A	9	SER	-	expression tag	UNP C3R9X4
A	10	GLY	-	expression tag	UNP C3R9X4
A	11	VAL	-	expression tag	UNP C3R9X4
A	12	ASP	-	expression tag	UNP C3R9X4
A	13	LEU	-	expression tag	UNP C3R9X4
A	14	GLY	-	expression tag	UNP C3R9X4
A	15	THR	-	expression tag	UNP C3R9X4
A	16	GLU	-	expression tag	UNP C3R9X4
A	17	ASN	-	expression tag	UNP C3R9X4
A	18	LEU	-	expression tag	UNP C3R9X4
A	19	TYR	-	expression tag	UNP C3R9X4
A	20	PHE	-	expression tag	UNP C3R9X4
A	21	GLN	-	expression tag	UNP C3R9X4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	-	expression tag	UNP C3R9X4
A	23	ASN	-	expression tag	UNP C3R9X4
B	1	MET	-	initiating methionine	UNP C3R9X4
B	2	HIS	-	expression tag	UNP C3R9X4
B	3	HIS	-	expression tag	UNP C3R9X4
B	4	HIS	-	expression tag	UNP C3R9X4
B	5	HIS	-	expression tag	UNP C3R9X4
B	6	HIS	-	expression tag	UNP C3R9X4
B	7	HIS	-	expression tag	UNP C3R9X4
B	8	SER	-	expression tag	UNP C3R9X4
B	9	SER	-	expression tag	UNP C3R9X4
B	10	GLY	-	expression tag	UNP C3R9X4
B	11	VAL	-	expression tag	UNP C3R9X4
B	12	ASP	-	expression tag	UNP C3R9X4
B	13	LEU	-	expression tag	UNP C3R9X4
B	14	GLY	-	expression tag	UNP C3R9X4
B	15	THR	-	expression tag	UNP C3R9X4
B	16	GLU	-	expression tag	UNP C3R9X4
B	17	ASN	-	expression tag	UNP C3R9X4
B	18	LEU	-	expression tag	UNP C3R9X4
B	19	TYR	-	expression tag	UNP C3R9X4
B	20	PHE	-	expression tag	UNP C3R9X4
B	21	GLN	-	expression tag	UNP C3R9X4
B	22	SER	-	expression tag	UNP C3R9X4
B	23	ASN	-	expression tag	UNP C3R9X4
C	1	MET	-	initiating methionine	UNP C3R9X4
C	2	HIS	-	expression tag	UNP C3R9X4
C	3	HIS	-	expression tag	UNP C3R9X4
C	4	HIS	-	expression tag	UNP C3R9X4
C	5	HIS	-	expression tag	UNP C3R9X4
C	6	HIS	-	expression tag	UNP C3R9X4
C	7	HIS	-	expression tag	UNP C3R9X4
C	8	SER	-	expression tag	UNP C3R9X4
C	9	SER	-	expression tag	UNP C3R9X4
C	10	GLY	-	expression tag	UNP C3R9X4
C	11	VAL	-	expression tag	UNP C3R9X4
C	12	ASP	-	expression tag	UNP C3R9X4
C	13	LEU	-	expression tag	UNP C3R9X4
C	14	GLY	-	expression tag	UNP C3R9X4
C	15	THR	-	expression tag	UNP C3R9X4
C	16	GLU	-	expression tag	UNP C3R9X4
C	17	ASN	-	expression tag	UNP C3R9X4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	LEU	-	expression tag	UNP C3R9X4
C	19	TYR	-	expression tag	UNP C3R9X4
C	20	PHE	-	expression tag	UNP C3R9X4
C	21	GLN	-	expression tag	UNP C3R9X4
C	22	SER	-	expression tag	UNP C3R9X4
C	23	ASN	-	expression tag	UNP C3R9X4
D	1	MET	-	initiating methionine	UNP C3R9X4
D	2	HIS	-	expression tag	UNP C3R9X4
D	3	HIS	-	expression tag	UNP C3R9X4
D	4	HIS	-	expression tag	UNP C3R9X4
D	5	HIS	-	expression tag	UNP C3R9X4
D	6	HIS	-	expression tag	UNP C3R9X4
D	7	HIS	-	expression tag	UNP C3R9X4
D	8	SER	-	expression tag	UNP C3R9X4
D	9	SER	-	expression tag	UNP C3R9X4
D	10	GLY	-	expression tag	UNP C3R9X4
D	11	VAL	-	expression tag	UNP C3R9X4
D	12	ASP	-	expression tag	UNP C3R9X4
D	13	LEU	-	expression tag	UNP C3R9X4
D	14	GLY	-	expression tag	UNP C3R9X4
D	15	THR	-	expression tag	UNP C3R9X4
D	16	GLU	-	expression tag	UNP C3R9X4
D	17	ASN	-	expression tag	UNP C3R9X4
D	18	LEU	-	expression tag	UNP C3R9X4
D	19	TYR	-	expression tag	UNP C3R9X4
D	20	PHE	-	expression tag	UNP C3R9X4
D	21	GLN	-	expression tag	UNP C3R9X4
D	22	SER	-	expression tag	UNP C3R9X4
D	23	ASN	-	expression tag	UNP C3R9X4

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0

- Molecule 3 is water.

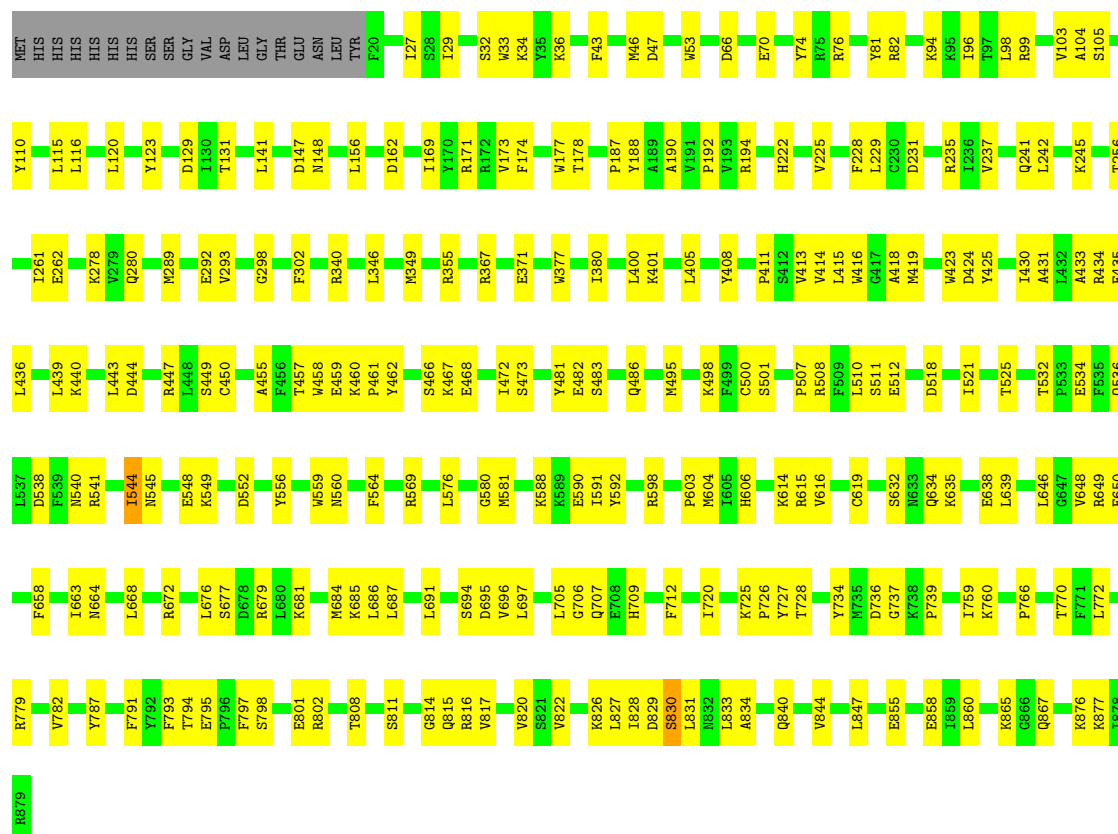
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total 98	O 98	0	0
3	B	123	Total 123	O 123	0	0
3	C	80	Total 80	O 80	0	0
3	D	70	Total 70	O 70	0	0

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.

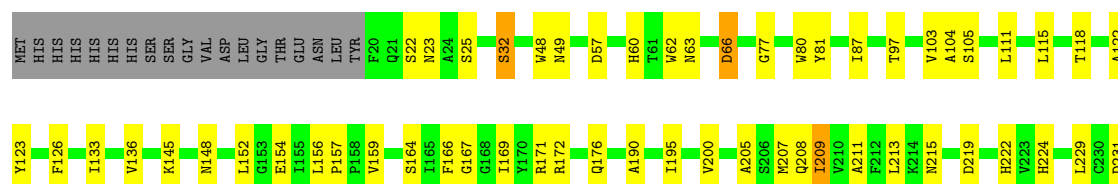
- Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

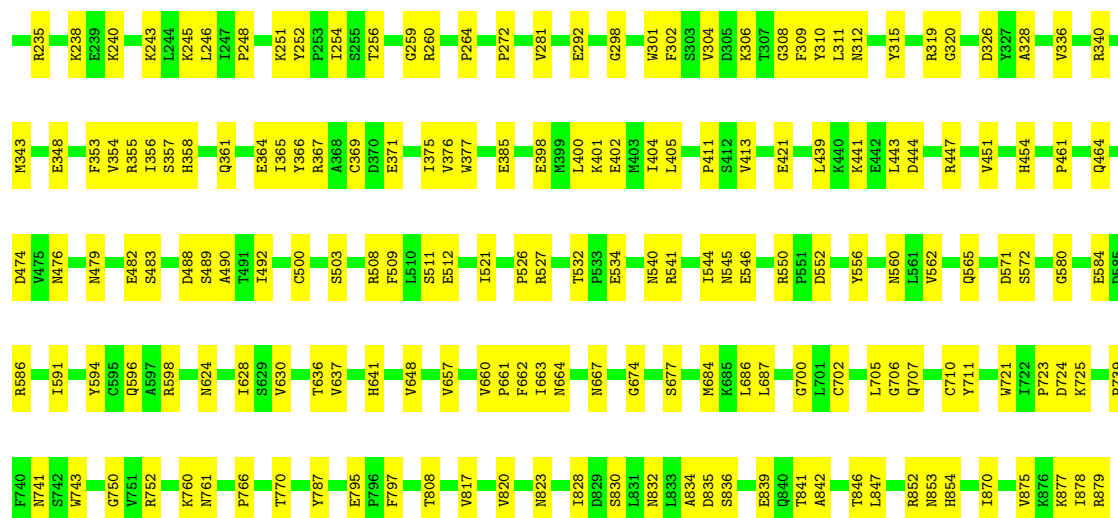
Chain A: 



- Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

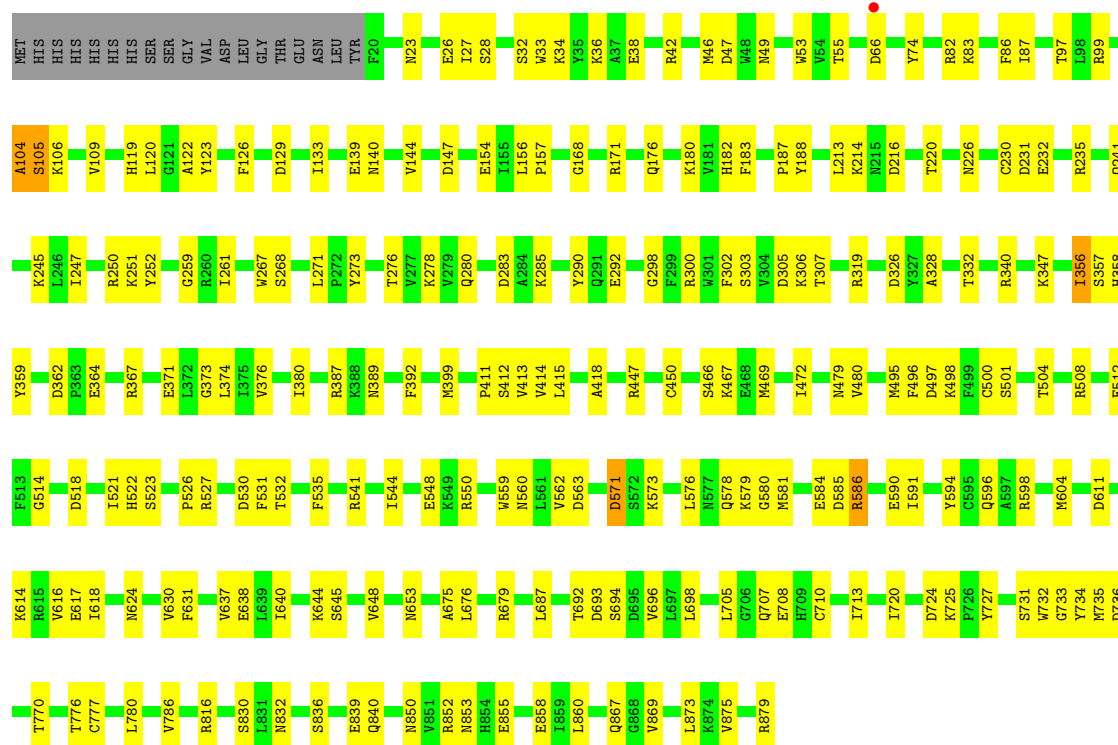
Chain B: 





• Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

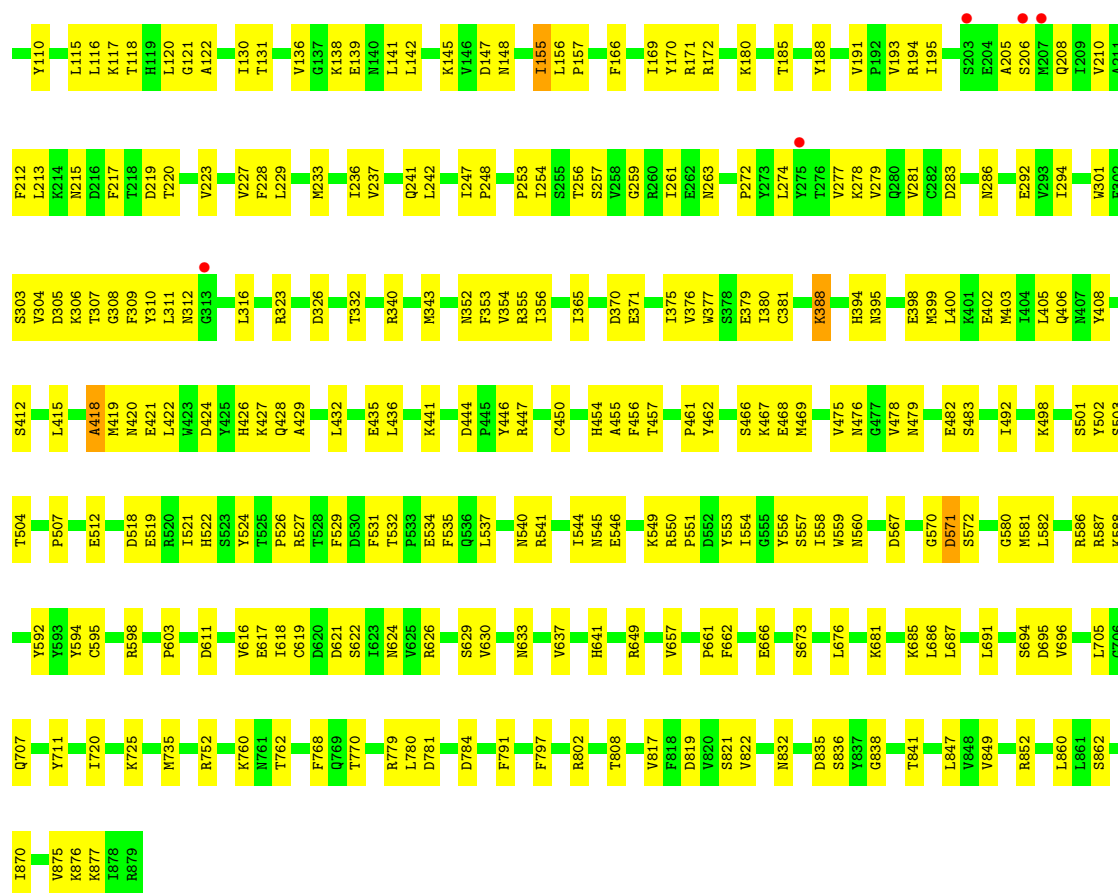
Chain C: 72% 25%



• Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

Chain D: 65% 33%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	242.66Å 101.36Å 168.60Å 90.00° 94.97° 90.00°	Depositor
Resolution (Å)	29.54 – 2.90 29.54 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.54-2.90) 99.4 (29.54-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.178 , 0.268 0.180 , 0.270	Depositor DCC
R_{free} test set	1988 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27956	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.46% 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

5.1 Standard geometry

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

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	0.40	0/7071	0.61	2/9580 (0.0%)
1	B	0.42	0/7084	0.64	0/9596
1	C	0.39	0/7079	0.60	0/9592
1	D	0.39	1/7027 (0.0%)	0.61	0/9532
All	All	0.40	1/28261 (0.0%)	0.61	2/38300 (0.0%)

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	D	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	263	ASN	C-O	5.11	1.26	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ALA	CA-C-N	5.27	130.74	123.04
1	A	104	ALA	C-N-CA	5.27	130.74	123.04

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	223	VAL	Peptide
1	D	303	SER	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	6901	0	6764	160	2
1	B	6914	0	6771	147	0
1	C	6909	0	6760	164	0
1	D	6857	0	6660	193	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	98	0	0	6	0
3	B	123	0	0	6	0
3	C	80	0	0	7	0
3	D	70	0	0	9	0
All	All	27956	0	26955	652	2

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 12.

All (652) 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:668:LEU:HD12	1:A:681:LYS:HG2	1.50	0.93
1:B:159:VAL:HG11	1:B:385:GLU:HG2	1.50	0.93
1:D:617:GLU:OE1	1:D:626:ARG:NH1	2.07	0.86
1:D:220:THR:HG22	1:D:247:ILE:HA	1.58	0.86
1:B:852:ARG:NH1	1:C:292:GLU:OE1	2.10	0.85
1:D:316:LEU:HD21	1:D:352:ASN:HD21	1.43	0.84
1:B:292:GLU:OE1	1:C:852:ARG:NH2	2.12	0.82
1:B:340:ARG:NH2	1:B:371:GLU:OE2	2.13	0.82
1:D:779:ARG:NH1	1:D:781:ASP:OD1	2.14	0.81
1:A:820:VAL:HG22	1:A:828:ILE:HB	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:649:ARG:NH1	3:D:1001:HOH:O	2.13	0.80
1:B:503:SER:O	1:B:508:ARG:NH1	2.15	0.80
1:D:694:SER:HB3	1:D:696:VAL:HG12	1.63	0.79
1:C:581:MET:HE1	1:C:591:ILE:HG13	1.65	0.78
1:D:817:VAL:HG22	1:D:832:ASN:HB2	1.67	0.77
1:B:231:ASP:HB3	1:B:235:ARG:H	1.50	0.76
1:B:97:THR:HG23	1:B:176:GLN:HG3	1.66	0.76
1:D:306:LYS:NZ	1:D:504:THR:O	2.15	0.76
1:D:626:ARG:HH11	1:D:626:ARG:HG3	1.49	0.75
1:C:616:VAL:HG23	1:C:720:ILE:HD12	1.69	0.75
1:D:326:ASP:O	1:D:586:ARG:NH2	2.19	0.75
1:B:421:GLU:HG2	1:B:454:HIS:HB3	1.69	0.74
1:C:638:GLU:HB2	1:C:648:VAL:HG22	1.70	0.72
1:D:278:LYS:HD3	1:D:294:ILE:HG22	1.71	0.72
1:C:640:ILE:HA	1:C:645:SER:HA	1.72	0.70
1:B:156:LEU:HD12	1:B:157:PRO:HD2	1.73	0.70
1:B:820:VAL:HG22	1:B:828:ILE:HB	1.73	0.70
1:D:156:LEU:HD12	1:D:157:PRO:HD2	1.72	0.70
1:D:172:ARG:NH2	3:D:1007:HOH:O	2.25	0.70
1:A:449:SER:HB3	1:A:473:SER:HB3	1.74	0.69
1:A:802:ARG:HG2	1:A:808:THR:HG21	1.75	0.69
1:C:230:CYS:HB2	1:C:276:THR:HG22	1.73	0.69
1:D:102:GLY:HA3	1:D:171:ARG:HG3	1.73	0.68
1:D:215:ASN:HD21	1:D:217:PHE:HB2	1.58	0.68
1:D:797:PHE:O	1:D:802:ARG:NH1	2.26	0.68
1:B:706:GLY:HA2	1:B:739:PRO:HB3	1.76	0.68
1:C:47:ASP:O	3:C:1002:HOH:O	2.12	0.68
1:B:66:ASP:OD1	3:B:1002:HOH:O	2.12	0.68
1:D:621:ASP:OD1	1:D:622:SER:N	2.24	0.68
1:D:760:LYS:HB3	1:D:841:THR:HG22	1.73	0.68
1:A:816:ARG:NH1	1:A:867:GLN:O	2.27	0.67
1:C:303:SER:OG	3:C:1001:HOH:O	2.10	0.67
1:D:340:ARG:NH2	1:D:371:GLU:OE1	2.28	0.67
1:B:209:ILE:HG12	1:B:256:THR:HG22	1.76	0.67
1:A:105:SER:HB2	1:A:147:ASP:O	1.95	0.67
1:B:546:GLU:O	1:B:550:ARG:HG3	1.95	0.67
1:B:641:HIS:HE1	1:B:661:PRO:O	1.78	0.67
1:D:256:THR:HG22	1:D:257:SER:H	1.60	0.67
1:B:264:PRO:O	3:B:1003:HOH:O	2.13	0.66
1:D:521:ILE:HG22	1:D:532:THR:HG22	1.77	0.66
1:D:616:VAL:HG23	1:D:720:ILE:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ASP:OD2	3:B:1001:HOH:O	2.12	0.66
1:C:42:ARG:HG3	1:C:42:ARG:HH11	1.60	0.66
1:A:355:ARG:HH12	1:A:512:GLU:HG3	1.61	0.66
1:A:604:MET:HE2	1:A:632:SER:HA	1.78	0.66
1:C:319:ARG:NH1	1:C:548:GLU:OE2	2.28	0.66
1:A:614:LYS:HG3	1:A:720:ILE:HD11	1.78	0.65
1:B:356:ILE:HG23	1:B:361:GLN:HG3	1.77	0.65
1:C:326:ASP:HB3	1:C:332:THR:HG22	1.78	0.65
1:C:544:ILE:HG21	1:C:598:ARG:HE	1.61	0.65
1:A:663:ILE:HD12	1:A:664:ASN:O	1.96	0.65
1:D:518:ASP:HB3	1:D:521:ILE:HD12	1.77	0.65
1:A:280:GLN:HB3	1:A:289:MET:HE2	1.79	0.65
1:A:431:ALA:O	1:A:435:GLU:HG3	1.96	0.65
1:A:706:GLY:HA2	1:A:739:PRO:HB3	1.79	0.65
1:B:123:TYR:O	1:B:171:ARG:NH2	2.30	0.64
1:B:527:ARG:NH1	3:B:1006:HOH:O	2.30	0.64
1:D:570:GLY:O	3:D:1002:HOH:O	2.15	0.64
1:D:377:TRP:CE3	1:D:415:LEU:HD13	2.32	0.64
1:A:129:ASP:OD1	1:A:131:THR:HG22	1.98	0.64
1:B:761:ASN:HB3	1:B:842:ALA:HB3	1.79	0.63
1:A:123:TYR:O	1:A:171:ARG:NH2	2.31	0.63
1:A:615:ARG:HB2	1:A:684:MET:HE2	1.80	0.63
1:C:598:ARG:HH12	1:C:653:ASN:HA	1.62	0.63
1:B:343:MET:HE3	1:B:365:ILE:HD11	1.81	0.62
1:C:630:VAL:HG11	1:C:637:VAL:HG21	1.82	0.62
1:D:227:VAL:HG22	1:D:279:VAL:HG22	1.81	0.62
1:D:526:PRO:HG3	1:D:534:GLU:HB3	1.82	0.62
1:C:120:LEU:HB3	1:C:156:LEU:HD13	1.79	0.62
1:A:298:GLY:N	1:A:411:PRO:HG3	2.15	0.62
1:A:619:CYS:HB3	1:A:686:LEU:HD22	1.82	0.62
1:B:641:HIS:NE2	1:B:667:ASN:OD1	2.33	0.62
1:C:105:SER:H	1:C:122:ALA:HA	1.65	0.62
1:D:483:SER:HB2	1:D:492:ILE:HD11	1.82	0.62
1:A:340:ARG:NH2	1:A:371:GLU:OE2	2.32	0.62
1:A:603:PRO:HB2	1:A:676:LEU:HD11	1.81	0.62
1:D:155:ILE:O	1:D:395:ASN:ND2	2.33	0.62
1:D:194:ARG:H	1:D:194:ARG:HD2	1.64	0.62
1:A:826:LYS:NZ	3:A:1001:HOH:O	2.15	0.61
1:C:154:GLU:HG3	1:C:389:ASN:HD21	1.65	0.61
1:D:205:ALA:HB3	1:D:261:ILE:HB	1.82	0.61
1:D:498:LYS:O	1:D:501:SER:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:541:ARG:HB2	1:D:594:TYR:OH	2.01	0.61
1:A:408:TYR:HE1	1:A:444:ASP:HB2	1.63	0.61
1:A:829:ASP:O	1:A:830:SER:HB3	2.00	0.61
1:C:579:LYS:NZ	3:C:1007:HOH:O	2.34	0.61
1:C:245:LYS:HE3	1:C:247:ILE:HD11	1.81	0.61
1:C:705:LEU:HD11	1:C:873:LEU:HB2	1.82	0.61
1:C:596:GLN:HB3	1:C:604:MET:HE3	1.82	0.61
1:A:43:PHE:O	1:A:82:ARG:NH2	2.34	0.61
1:D:191:VAL:O	1:D:194:ARG:NH1	2.34	0.61
1:B:545:ASN:OD1	1:B:598:ARG:NH1	2.32	0.61
1:D:519:GLU:OE1	3:D:1003:HOH:O	2.16	0.61
1:D:603:PRO:HB2	1:D:676:LEU:HD11	1.84	0.60
1:D:540:ASN:O	1:D:544:ILE:HG12	2.02	0.60
1:D:309:PHE:HB2	1:D:554:ILE:HB	1.82	0.60
1:D:304:VAL:HG22	1:D:507:PRO:HG3	1.82	0.60
1:D:502:TYR:O	1:D:504:THR:N	2.34	0.60
1:D:381:CYS:SG	1:D:399:MET:HE1	2.41	0.60
1:D:305:ASP:CG	1:D:307:THR:HG22	2.26	0.60
1:A:569:ARG:NH2	3:A:1009:HOH:O	2.35	0.60
1:A:590:GLU:OE2	1:A:606:HIS:NE2	2.25	0.60
1:B:22:SER:HB3	1:C:850:ASN:O	2.00	0.60
1:B:707:GLN:HE21	1:B:770:THR:HG21	1.66	0.60
1:B:479:ASN:OD1	1:B:511:SER:HB2	2.02	0.59
1:B:401:LYS:HG2	1:B:443:LEU:HD11	1.83	0.59
1:D:427:LYS:HD3	1:D:427:LYS:N	2.17	0.59
1:B:172:ARG:NH2	3:B:1011:HOH:O	2.35	0.59
1:C:280:GLN:HG2	1:C:292:GLU:HG3	1.84	0.59
1:D:546:GLU:O	1:D:550:ARG:HD2	2.01	0.59
1:B:376:VAL:HB	1:B:413:VAL:HA	1.83	0.59
1:B:741:ASN:ND2	1:B:750:GLY:HA2	2.18	0.59
1:C:86:PHE:CE1	1:C:139:GLU:HB2	2.38	0.59
1:D:85:LEU:HD22	1:D:142:LEU:HD22	1.85	0.59
1:B:306:LYS:O	1:B:552:ASP:HA	2.03	0.59
1:B:367:ARG:NH2	1:C:698:LEU:O	2.34	0.59
1:B:560:ASN:O	1:B:580:GLY:HA2	2.03	0.59
1:D:415:LEU:HD22	1:D:450:CYS:HB3	1.84	0.59
1:C:500:CYS:HB3	1:C:508:ARG:HH21	1.66	0.59
1:D:191:VAL:HG23	1:D:405:LEU:O	2.03	0.58
1:A:96:ILE:H	1:A:131:THR:HB	1.68	0.58
1:C:617:GLU:OE2	1:C:624:ASN:ND2	2.34	0.58
1:A:639:LEU:HD23	1:A:646:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:HIS:NE2	1:A:245:LYS:HD2	2.18	0.58
1:C:725:LYS:HE2	1:C:732:TRP:O	2.04	0.58
1:B:461:PRO:HA	1:B:464:GLN:HG3	1.85	0.58
1:A:759:ILE:HD12	1:A:794:THR:HG21	1.86	0.58
1:C:66:ASP:HB3	1:C:74:TYR:HB2	1.86	0.58
1:D:219:ASP:O	1:D:248:PRO:HG3	2.04	0.58
1:C:512:GLU:HB2	1:C:559:TRP:HB2	1.85	0.57
1:C:387:ARG:HB2	1:C:392:PHE:CD1	2.39	0.57
1:D:526:PRO:HB2	1:D:535:PHE:HB2	1.86	0.57
1:B:710:CYS:O	1:B:723:PRO:HG3	2.05	0.57
1:A:638:GLU:HB2	1:A:648:VAL:HG22	1.86	0.57
1:C:226:ASN:OD1	1:C:241:GLN:NE2	2.33	0.57
1:B:482:GLU:O	1:B:483:SER:HB3	2.04	0.57
1:D:236:ILE:HD12	1:D:236:ILE:H	1.69	0.57
1:B:852:ARG:NH2	1:C:23:ASN:OD1	2.38	0.57
1:D:67:VAL:HG13	1:D:567:ASP:HB2	1.86	0.57
1:A:518:ASP:HB3	1:A:521:ILE:HD12	1.86	0.56
1:B:630:VAL:HG11	1:B:637:VAL:HG21	1.86	0.56
1:D:80:TRP:CE2	1:D:145:LYS:HG3	2.40	0.56
1:A:588:LYS:HD3	1:A:592:TYR:CE2	2.40	0.56
1:B:795:GLU:HB3	1:B:839:GLU:HA	1.86	0.56
1:A:498:LYS:O	1:A:501:SER:HB2	2.06	0.56
1:A:634:GLN:HB3	3:A:1039:HOH:O	2.04	0.56
1:A:74:TYR:CE1	1:A:76:ARG:HD3	2.41	0.56
1:A:798:SER:OG	1:A:801:GLU:HG3	2.05	0.56
1:B:105:SER:H	1:B:122:ALA:HB2	1.71	0.56
1:B:115:LEU:HD11	1:B:118:THR:HG22	1.88	0.56
1:B:817:VAL:HG22	1:B:832:ASN:HB2	1.85	0.56
1:C:526:PRO:O	1:C:527:ARG:HD3	2.06	0.56
1:C:531:PHE:CZ	1:C:571:ASP:HB3	2.41	0.56
1:C:694:SER:HB3	1:C:696:VAL:HG12	1.88	0.56
1:D:603:PRO:HA	1:D:633:ASN:HD22	1.70	0.56
1:A:466:SER:OG	1:A:467:LYS:N	2.38	0.56
1:B:238:LYS:HZ3	1:B:260:ARG:HG3	1.71	0.56
1:D:791:PHE:CE2	1:D:847:LEU:HD12	2.41	0.56
1:A:34:LYS:HD2	1:A:53:TRP:HB2	1.87	0.56
1:A:791:PHE:O	1:A:844:VAL:HA	2.05	0.56
1:A:36:LYS:HE3	1:A:53:TRP:CD1	2.41	0.55
1:A:538:ASP:OD2	1:A:541:ARG:NH1	2.39	0.55
1:A:787:TYR:CZ	1:A:877:LYS:HG3	2.41	0.55
1:C:34:LYS:HD3	1:C:55:THR:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ASP:OD1	1:D:148:ASN:N	2.39	0.55
1:A:440:LYS:HD2	1:A:449:SER:OG	2.06	0.55
1:C:119:HIS:CD2	1:C:126:PHE:HB3	2.41	0.55
1:A:726:PRO:HG3	1:A:734:TYR:CZ	2.42	0.55
1:C:479:ASN:CG	1:C:512:GLU:HG2	2.32	0.55
1:A:649:ARG:HG3	1:A:658:PHE:CE1	2.41	0.55
1:B:208:GLN:NE2	1:B:256:THR:O	2.39	0.55
1:A:672:ARG:HG2	1:A:677:SER:HB3	1.88	0.55
1:B:377:TRP:HZ3	1:B:509:PHE:CD1	2.25	0.55
1:A:811:SER:O	1:A:814:GLY:N	2.24	0.55
1:D:705:LEU:HD12	1:D:870:ILE:HG12	1.88	0.55
1:A:616:VAL:HG22	1:A:685:LYS:HB3	1.89	0.55
1:A:725:LYS:HZ3	1:A:728:THR:HG22	1.72	0.55
1:D:316:LEU:HD21	1:D:352:ASN:ND2	2.19	0.54
1:C:305:ASP:OD1	1:C:307:THR:HG22	2.08	0.54
1:C:340:ARG:NH2	1:C:371:GLU:OE2	2.40	0.54
1:D:618:ILE:HD13	1:D:725:LYS:HE3	1.90	0.54
1:D:832:ASN:O	1:D:836:SER:HB2	2.07	0.54
1:A:99:ARG:HD3	1:A:174:PHE:HB2	1.90	0.54
1:A:705:LEU:HB3	1:A:772:LEU:HD12	1.89	0.54
1:C:133:ILE:H	1:C:133:ILE:HD12	1.72	0.54
1:A:436:LEU:O	1:A:440:LYS:HG3	2.07	0.53
1:B:77:GLY:H	1:B:148:ASN:HB3	1.73	0.53
1:C:736:ASP:OD2	1:C:776:THR:OG1	2.26	0.53
1:A:192:PRO:HG2	1:A:293:VAL:HG11	1.89	0.53
1:A:33:TRP:CE3	1:A:81:TYR:HB3	2.42	0.53
1:D:311:LEU:HD13	1:D:375:ILE:HD11	1.90	0.53
1:D:466:SER:OG	1:D:467:LYS:N	2.41	0.53
1:D:544:ILE:HD12	1:D:556:TYR:CE2	2.43	0.53
1:A:103:VAL:HG22	1:A:169:ILE:HG23	1.91	0.53
1:A:736:ASP:OD1	1:A:737:GLY:N	2.42	0.53
1:D:305:ASP:OD1	1:D:307:THR:HG22	2.09	0.53
1:B:80:TRP:CE2	1:B:145:LYS:HG3	2.44	0.53
1:B:677:SER:HB3	1:C:679:ARG:HH22	1.74	0.53
1:C:415:LEU:HB3	1:C:450:CYS:SG	2.49	0.53
1:C:526:PRO:HB2	1:C:535:PHE:HB2	1.90	0.53
1:D:469:MET:SD	1:D:469:MET:N	2.81	0.53
1:A:120:LEU:HB3	1:A:156:LEU:HD13	1.90	0.53
1:A:541:ARG:NH1	3:A:1002:HOH:O	2.42	0.53
1:A:725:LYS:NZ	1:A:728:THR:HG22	2.23	0.53
1:B:62:TRP:HZ2	1:B:148:ASN:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:ILE:HD11	1:D:400:LEU:HD12	1.91	0.53
1:D:394:HIS:O	1:D:398:GLU:HG2	2.09	0.53
1:B:308:GLY:HA3	1:B:315:TYR:HE1	1.74	0.52
1:D:784:ASP:O	1:D:877:LYS:NZ	2.41	0.52
1:D:63:ASN:HA	1:D:66:ASP:HB2	1.91	0.52
1:A:228:PHE:HB2	1:A:278:LYS:HB3	1.92	0.52
1:C:523:SER:HB2	1:C:532:THR:HG21	1.91	0.52
1:C:541:ARG:HG2	1:C:594:TYR:OH	2.09	0.52
1:D:518:ASP:OD1	1:D:572:SER:OG	2.27	0.52
1:B:677:SER:HB3	1:C:679:ARG:HH12	1.74	0.52
1:B:238:LYS:NZ	1:B:260:ARG:HG3	2.24	0.52
1:C:376:VAL:HB	1:C:413:VAL:HA	1.91	0.52
1:D:415:LEU:HB3	1:D:450:CYS:SG	2.49	0.52
1:A:29:ILE:HD11	1:A:173:VAL:HG12	1.92	0.52
1:A:424:ASP:OD1	1:A:460:LYS:HE3	2.10	0.52
1:C:562:VAL:HG11	1:C:586:ARG:NH1	2.24	0.52
1:D:90:GLU:HG3	1:D:90:GLU:O	2.10	0.52
1:D:256:THR:HG22	1:D:257:SER:N	2.24	0.52
1:D:307:THR:HG23	1:D:310:TYR:OH	2.10	0.52
1:C:42:ARG:HG3	1:C:42:ARG:NH1	2.25	0.52
1:C:97:THR:HG22	1:C:129:ASP:HA	1.91	0.52
1:A:815:GLN:OE1	1:A:865:LYS:NZ	2.41	0.52
1:D:45:SER:HB2	1:D:48:TRP:HB2	1.91	0.52
1:D:208:GLN:HA	1:D:257:SER:HA	1.91	0.52
1:A:298:GLY:H	1:A:411:PRO:HG3	1.75	0.52
1:A:822:VAL:HG12	1:A:827:LEU:HD23	1.92	0.52
1:A:222:HIS:CE1	1:A:245:LYS:HD2	2.45	0.51
1:B:846:THR:C	1:B:847:LEU:HD12	2.35	0.51
1:C:497:ASP:OD1	1:C:550:ARG:NH1	2.42	0.51
1:D:529:PHE:HB3	1:D:752:ARG:HD2	1.93	0.51
1:A:377:TRP:NE1	1:A:450:CYS:HG	2.09	0.51
1:B:224:HIS:ND1	1:B:243:LYS:HG2	2.25	0.51
1:A:581:MET:HE3	1:A:591:ILE:HG23	1.91	0.51
1:B:104:ALA:HB3	1:B:167:GLY:HA2	1.92	0.51
1:D:274:LEU:HD21	1:D:370:ASP:HB2	1.93	0.51
1:C:527:ARG:NH2	3:C:1008:HOH:O	2.42	0.51
1:D:707:GLN:HB2	1:D:770:THR:HG21	1.92	0.51
1:A:76:ARG:NE	1:A:148:ASN:O	2.40	0.51
1:A:413:VAL:HG11	1:A:416:TRP:CH2	2.46	0.51
1:D:105:SER:HB2	1:D:147:ASP:O	2.11	0.51
1:C:585:ASP:O	1:C:586:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:694:SER:C	1:C:696:VAL:H	2.19	0.51
1:D:304:VAL:HG22	1:D:507:PRO:CG	2.41	0.51
1:A:408:TYR:CE1	1:A:444:ASP:HB2	2.45	0.51
1:A:481:TYR:OH	1:A:512:GLU:OE2	2.29	0.51
1:D:421:GLU:HG3	1:D:479:ASN:ND2	2.26	0.51
1:B:319:ARG:HG2	1:B:556:TYR:CE1	2.46	0.50
1:B:328:ALA:HB2	1:B:584:GLU:HG3	1.93	0.50
1:D:215:ASN:ND2	1:D:217:PHE:HB2	2.25	0.50
1:A:510:LEU:HB3	1:A:556:TYR:CB	2.41	0.50
1:B:320:GLY:HA3	1:B:353:PHE:O	2.11	0.50
1:B:521:ILE:HG22	1:B:532:THR:HG22	1.92	0.50
1:D:457:THR:HA	1:D:462:TYR:CD2	2.46	0.50
1:B:636:THR:HG23	1:B:648:VAL:HG13	1.93	0.50
1:C:105:SER:O	3:C:1003:HOH:O	2.20	0.50
1:C:560:ASN:O	1:C:580:GLY:HA2	2.11	0.50
1:C:692:THR:OG1	1:C:693:ASP:OD1	2.28	0.50
1:D:105:SER:H	1:D:122:ALA:HB2	1.77	0.50
1:D:432:LEU:HA	1:D:435:GLU:OE1	2.11	0.50
1:A:27:ILE:HG22	1:A:177:TRP:HZ3	1.77	0.50
1:A:791:PHE:HB3	1:A:793:PHE:CE2	2.47	0.50
1:A:827:LEU:HG	1:A:847:LEU:HD22	1.94	0.50
1:C:816:ARG:HD3	1:C:867:GLN:O	2.12	0.50
1:D:624:ASN:O	1:D:662:PHE:HB2	2.12	0.50
1:B:398:GLU:O	1:B:402:GLU:HG3	2.11	0.49
1:B:400:LEU:HD23	1:B:439:LEU:HD23	1.93	0.49
1:C:214:LYS:HE2	1:C:251:LYS:HG2	1.93	0.49
1:A:70:GLU:CD	1:A:760:LYS:HG2	2.37	0.49
1:B:87:ILE:HG22	1:B:136:VAL:HG13	1.94	0.49
1:D:229:LEU:O	1:D:237:VAL:HG22	2.12	0.49
1:A:532:THR:HB	1:A:534:GLU:OE1	2.11	0.49
1:D:819:ASP:HB2	1:D:862:SER:OG	2.12	0.49
1:C:816:ARG:HD2	1:C:869:VAL:HG22	1.95	0.49
1:D:82:ARG:NH2	1:D:141:LEU:HD21	2.27	0.49
1:A:380:ILE:HG13	1:A:418:ALA:HA	1.94	0.49
1:A:110:TYR:CE2	1:A:115:LEU:HB2	2.47	0.49
1:B:164:SER:HB2	1:B:166:PHE:CE1	2.47	0.49
1:C:267:TRP:CH2	1:C:412:SER:HA	2.48	0.49
1:D:549:LYS:O	1:D:551:PRO:HD3	2.12	0.49
1:B:211:ALA:HB3	1:B:254:ILE:HD11	1.95	0.49
1:D:180:LYS:HB2	1:D:217:PHE:CE2	2.47	0.49
1:C:180:LYS:HB3	1:C:216:ASP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:MET:HE2	1:D:422:LEU:HD11	1.93	0.49
1:A:794:THR:HG23	1:A:840:GLN:HA	1.95	0.49
1:C:306:LYS:NZ	1:C:504:THR:O	2.42	0.49
1:B:103:VAL:HG22	1:B:126:PHE:HE2	1.78	0.48
1:B:444:ASP:OD2	1:B:447:ARG:HD2	2.13	0.48
1:B:664:ASN:HB2	1:B:686:LEU:HD12	1.95	0.48
1:D:278:LYS:HD3	1:D:294:ILE:CG2	2.42	0.48
1:A:261:ILE:O	1:A:262:GLU:HB2	2.14	0.48
1:A:614:LYS:HG3	1:A:720:ILE:CD1	2.42	0.48
1:B:663:ILE:HD12	1:B:664:ASN:O	2.12	0.48
1:C:518:ASP:HB3	1:C:521:ILE:HD12	1.94	0.48
1:D:629:SER:HB3	1:D:657:VAL:HG22	1.94	0.48
1:B:246:LEU:HA	1:B:252:TYR:CE2	2.47	0.48
1:C:123:TYR:O	1:C:171:ARG:NH2	2.45	0.48
1:C:171:ARG:HD2	1:C:362:ASP:OD1	2.14	0.48
1:C:298:GLY:N	1:C:411:PRO:HG3	2.27	0.48
1:C:644:LYS:HA	1:C:644:LYS:HD3	1.49	0.48
1:B:308:GLY:HA3	1:B:315:TYR:CE1	2.48	0.48
1:D:832:ASN:ND2	3:D:1019:HOH:O	2.47	0.48
1:A:229:LEU:O	1:A:237:VAL:HG22	2.13	0.48
1:C:498:LYS:O	1:C:501:SER:HB3	2.12	0.48
1:C:713:ILE:HG13	1:C:720:ILE:HG12	1.94	0.48
1:D:117:LYS:HG3	1:D:118:THR:N	2.28	0.48
1:D:283:ASP:HB3	1:D:286:ASN:HB3	1.93	0.48
1:D:581:MET:HE1	1:D:595:CYS:SG	2.53	0.48
1:D:821:SER:HB2	1:D:860:LEU:HD12	1.95	0.48
1:A:423:TRP:O	1:A:460:LYS:HB2	2.13	0.48
1:D:279:VAL:O	1:D:292:GLU:HA	2.13	0.48
1:D:630:VAL:HG11	1:D:637:VAL:HG11	1.94	0.48
1:A:560:ASN:O	1:A:580:GLY:HA2	2.14	0.48
1:A:817:VAL:HA	1:A:831:LEU:O	2.14	0.48
1:D:388:LYS:HE3	1:D:428:GLN:OE1	2.14	0.48
1:D:419:MET:HE2	1:D:422:LEU:CD1	2.44	0.48
1:A:457:THR:HG21	1:A:498:LYS:HD3	1.96	0.48
1:B:103:VAL:HG12	1:B:169:ILE:HG23	1.96	0.48
1:B:152:LEU:C	1:B:154:GLU:H	2.20	0.48
1:D:106:LYS:HG3	1:D:120:LEU:HD23	1.95	0.48
1:D:110:TYR:CE2	1:D:115:LEU:HB2	2.49	0.48
1:D:195:ILE:CD1	1:D:277:VAL:HG11	2.43	0.48
1:D:822:VAL:HG11	1:D:849:VAL:HG21	1.96	0.48
1:A:355:ARG:NH1	1:A:512:GLU:HG3	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ILE:HD12	1:C:140:ASN:ND2	2.29	0.48
1:D:308:GLY:C	1:D:554:ILE:HG22	2.39	0.48
1:B:25:SER:HB2	1:C:850:ASN:HD21	1.79	0.47
1:D:522:HIS:NE2	1:D:611:ASP:OD2	2.38	0.47
1:D:666:GLU:OE2	1:D:681:LYS:HD3	2.14	0.47
1:A:468:GLU:HG2	1:D:446:TYR:OH	2.14	0.47
1:B:105:SER:H	1:B:122:ALA:CB	2.27	0.47
1:C:522:HIS:NE2	1:C:611:ASP:OD2	2.35	0.47
1:D:355:ARG:NE	1:D:379:GLU:OE2	2.43	0.47
1:D:524:TYR:CE1	1:D:626:ARG:NH1	2.83	0.47
1:B:624:ASN:O	1:B:662:PHE:HB2	2.14	0.47
1:D:193:VAL:HG23	1:D:210:VAL:O	2.14	0.47
1:C:356:ILE:HG12	1:C:376:VAL:HG13	1.96	0.47
1:A:797:PHE:HB3	1:A:801:GLU:HB2	1.96	0.47
1:B:60:HIS:ND1	1:B:81:TYR:OH	2.40	0.47
1:B:172:ARG:NH2	1:B:336:VAL:HG21	2.30	0.47
1:B:355:ARG:NH1	1:B:512:GLU:HG3	2.30	0.47
1:D:685:LYS:HE3	1:D:687:LEU:HD21	1.95	0.47
1:A:355:ARG:NH1	1:A:511:SER:HB2	2.30	0.47
1:C:231:ASP:HB3	1:C:235:ARG:H	1.80	0.47
1:C:347:LYS:HB2	1:C:374:LEU:HD11	1.97	0.47
1:A:455:ALA:HB1	1:A:495:MET:HE2	1.95	0.47
1:A:548:GLU:OE2	1:A:556:TYR:OH	2.25	0.47
1:B:62:TRP:CZ2	1:B:148:ASN:HB2	2.50	0.47
1:B:222:HIS:NE2	1:B:245:LYS:HG3	2.29	0.47
1:C:302:PHE:HZ	1:C:447:ARG:HA	1.80	0.47
1:D:380:ILE:HG13	1:D:418:ALA:HA	1.96	0.47
1:D:641:HIS:HE1	1:D:661:PRO:O	1.97	0.47
1:A:94:LYS:HB3	1:A:178:THR:O	2.15	0.47
1:B:364:GLU:OE1	1:B:367:ARG:NH1	2.44	0.47
1:B:500:CYS:HB3	1:B:508:ARG:NH2	2.29	0.47
1:B:705:LEU:HD12	1:B:870:ILE:HG12	1.95	0.47
1:B:832:ASN:OD1	1:B:835:ASP:HB2	2.14	0.47
1:B:853:ASN:OD1	1:B:854:HIS:N	2.48	0.47
1:A:419:MET:HE1	1:A:433:ALA:HB2	1.97	0.47
1:A:797:PHE:CG	1:A:808:THR:HG23	2.50	0.47
1:D:466:SER:OG	1:D:468:GLU:N	2.41	0.47
1:B:166:PHE:H	1:B:166:PHE:HD1	1.62	0.47
1:B:795:GLU:HG2	1:B:834:ALA:HB2	1.97	0.47
1:C:46:MET:HG2	3:C:1029:HOH:O	2.15	0.47
1:D:587:ARG:NH2	3:D:1003:HOH:O	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ARG:HH12	1:B:512:GLU:HG3	1.80	0.46
1:C:598:ARG:NH1	1:C:653:ASN:CA	2.78	0.46
1:C:614:LYS:HE3	1:C:614:LYS:HB3	1.81	0.46
1:D:376:VAL:HG23	1:D:412:SER:HB2	1.97	0.46
1:A:466:SER:OG	1:A:468:GLU:HG3	2.15	0.46
1:A:510:LEU:HB3	1:A:556:TYR:HB2	1.96	0.46
1:C:598:ARG:HH11	1:C:598:ARG:HG2	1.81	0.46
1:D:780:LEU:HD22	1:D:875:VAL:HG21	1.97	0.46
1:B:238:LYS:NZ	1:B:259:GLY:O	2.48	0.46
1:B:304:VAL:HG12	1:B:309:PHE:HD1	1.79	0.46
1:D:588:LYS:HD3	1:D:592:TYR:CE2	2.50	0.46
1:A:795:GLU:HG2	1:A:834:ALA:HB2	1.97	0.46
1:C:357:SER:HB2	1:C:358:HIS:ND1	2.31	0.46
1:A:46:MET:HA	1:A:141:LEU:HD22	1.98	0.46
1:C:26:GLU:OE2	1:C:99:ARG:NH1	2.49	0.46
1:C:66:ASP:HB3	1:C:74:TYR:CB	2.44	0.46
1:C:104:ALA:HB3	1:C:168:GLY:H	1.80	0.46
1:C:598:ARG:HH12	1:C:653:ASN:CA	2.26	0.46
1:D:797:PHE:CG	1:D:808:THR:HG22	2.50	0.46
1:C:300:ARG:HH22	1:C:302:PHE:HE1	1.63	0.46
1:A:120:LEU:HB3	1:A:156:LEU:CD1	2.46	0.46
1:A:280:GLN:HG2	1:A:292:GLU:HG3	1.98	0.46
1:C:86:PHE:CZ	1:C:139:GLU:HB2	2.50	0.46
1:D:46:MET:HA	1:D:141:LEU:HD22	1.98	0.46
1:D:617:GLU:HG2	1:D:711:TYR:CE1	2.51	0.46
1:A:415:LEU:HB3	1:A:450:CYS:SG	2.56	0.46
1:B:743:TRP:HZ3	1:B:752:ARG:O	1.99	0.46
1:C:708:GLU:OE2	1:C:734:TYR:OH	2.20	0.46
1:A:231:ASP:OD2	1:A:235:ARG:NH1	2.33	0.46
1:A:458:TRP:HZ2	1:A:486:GLN:NE2	2.14	0.46
1:C:594:TYR:CZ	1:C:598:ARG:HD2	2.51	0.46
1:A:367:ARG:NH1	3:A:1019:HOH:O	2.48	0.46
1:C:123:TYR:CG	1:C:359:TYR:HB2	2.51	0.46
1:D:402:GLU:HG2	1:D:406:GLN:NE2	2.31	0.46
1:A:190:ALA:HB2	1:A:405:LEU:HB3	1.98	0.45
1:A:302:PHE:CE2	1:A:414:VAL:HG13	2.50	0.45
1:A:797:PHE:CD2	1:A:808:THR:HG23	2.51	0.45
1:D:188:TYR:HD1	1:D:402:GLU:HG3	1.80	0.45
1:D:531:PHE:CZ	1:D:571:ASP:HB3	2.51	0.45
1:A:401:LYS:HG2	1:A:443:LEU:HD21	1.99	0.45
1:A:444:ASP:OD2	1:A:447:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:VAL:HG13	1:B:205:ALA:HB2	1.98	0.45
1:B:240:LYS:HD3	1:B:256:THR:OG1	2.17	0.45
1:C:36:LYS:HG2	1:C:38:GLU:HB3	1.98	0.45
1:C:389:ASN:HB2	1:C:392:PHE:HB2	1.96	0.45
1:D:241:GLN:C	1:D:242:LEU:HD23	2.41	0.45
1:D:444:ASP:OD2	1:D:447:ARG:NH1	2.42	0.45
1:D:432:LEU:O	1:D:436:LEU:HG	2.16	0.45
1:C:278:LYS:HD3	1:C:292:GLU:OE2	2.16	0.45
1:C:576:LEU:HD23	1:C:578:GLN:HG2	1.99	0.45
1:B:847:LEU:HG	1:C:27:ILE:HD12	1.99	0.45
1:C:853:ASN:HB3	1:C:855:GLU:HG3	1.97	0.45
1:D:355:ARG:NH2	1:D:420:ASN:OD1	2.50	0.45
1:A:697:LEU:HB3	1:A:877:LYS:HB2	1.98	0.45
1:B:272:PRO:HG2	3:B:1042:HOH:O	2.17	0.45
1:B:326:ASP:OD2	1:B:565:GLN:NE2	2.46	0.45
1:D:206:SER:HA	1:D:259:GLY:HA2	1.98	0.45
1:D:475:VAL:HG11	1:D:554:ILE:HD11	1.97	0.45
1:A:668:LEU:CD1	1:A:681:LYS:HE2	2.47	0.45
1:A:707:GLN:HE21	1:A:770:THR:HG21	1.81	0.45
1:B:878:ILE:O	1:B:879:ARG:HB3	2.17	0.45
1:C:544:ILE:CG2	1:C:598:ARG:HE	2.28	0.45
1:B:441:LYS:NZ	1:B:474:ASP:OD2	2.50	0.45
1:B:541:ARG:HG3	1:B:594:TYR:OH	2.16	0.45
1:C:182:HIS:CE1	1:C:214:LYS:HD2	2.52	0.45
1:D:558:ILE:HG21	1:D:581:MET:SD	2.57	0.45
1:A:545:ASN:OD1	1:A:598:ARG:NH1	2.23	0.45
1:A:635:LYS:NZ	3:A:1022:HOH:O	2.50	0.45
1:B:311:LEU:HD22	1:B:375:ILE:HD11	1.97	0.45
1:B:48:TRP:CG	1:B:49:ASN:H	2.35	0.44
1:B:171:ARG:HH12	1:B:361:GLN:HA	1.83	0.44
1:C:328:ALA:HB2	1:C:584:GLU:HG3	1.99	0.44
1:C:414:VAL:HG12	1:C:415:LEU:HD12	1.98	0.44
1:C:594:TYR:HB2	1:C:631:PHE:CE2	2.53	0.44
1:D:582:LEU:HD23	1:D:588:LYS:HA	1.99	0.44
1:A:687:LEU:HD21	1:A:696:VAL:HG21	1.99	0.44
1:C:106:LYS:HB3	1:C:147:ASP:HB3	1.98	0.44
1:C:154:GLU:HG3	1:C:154:GLU:O	2.17	0.44
1:A:242:LEU:HD11	1:A:256:THR:OG1	2.17	0.44
1:A:727:TYR:CE1	1:A:779:ARG:HB2	2.52	0.44
1:A:820:VAL:HG22	1:A:828:ILE:CB	2.40	0.44
1:C:469:MET:HA	1:C:472:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:TRP:CE2	1:B:312:ASN:HA	2.51	0.44
1:B:400:LEU:O	1:B:404:ILE:HG13	2.18	0.44
1:C:573:LYS:NZ	3:C:1009:HOH:O	2.43	0.44
1:D:103:VAL:HG22	1:D:169:ILE:HG23	1.99	0.44
1:A:545:ASN:O	1:A:549:LYS:HG2	2.17	0.44
1:C:268:SER:HB3	1:C:271:LEU:H	1.83	0.44
1:D:195:ILE:HD13	1:D:277:VAL:HG11	1.99	0.44
1:D:482:GLU:HB2	1:D:492:ILE:HG12	1.99	0.44
1:D:637:VAL:HA	1:D:673:SER:HB2	1.98	0.44
1:A:858:GLU:OE1	1:A:860:LEU:HD11	2.18	0.44
1:C:387:ARG:HB2	1:C:392:PHE:CG	2.53	0.44
1:A:444:ASP:OD2	1:A:447:ARG:HB2	2.17	0.44
1:C:278:LYS:HE2	1:C:278:LYS:HB2	1.63	0.44
1:B:213:LEU:HD21	1:B:281:VAL:HG21	2.00	0.44
1:C:562:VAL:HG12	1:C:563:ASP:O	2.18	0.44
1:D:838:GLY:O	1:D:841:THR:OG1	2.36	0.44
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.86	0.44
1:B:23:ASN:ND2	1:C:852:ARG:NH1	2.66	0.44
1:C:480:VAL:HG21	1:C:496:PHE:HE2	1.83	0.44
1:D:581:MET:HB3	1:D:581:MET:HE3	1.66	0.44
1:A:430:ILE:H	1:A:430:ILE:HG12	1.65	0.43
1:D:343:MET:HE1	1:D:354:VAL:HG21	2.00	0.43
1:A:540:ASN:ND2	1:A:591:ILE:HD11	2.33	0.43
1:B:302:PHE:HA	1:B:310:TYR:O	2.19	0.43
1:B:540:ASN:O	1:B:544:ILE:HD12	2.18	0.43
1:D:380:ILE:HG23	1:D:403:MET:SD	2.58	0.43
1:D:441:LYS:HA	1:D:444:ASP:O	2.18	0.43
1:C:187:PRO:HG2	1:C:188:TYR:CD2	2.54	0.43
1:D:56:VAL:HG11	1:D:60:HIS:CD2	2.54	0.43
1:D:304:VAL:HG21	1:D:475:VAL:HG22	2.01	0.43
1:D:559:TRP:HA	1:D:560:ASN:HA	1.74	0.43
1:A:340:ARG:HE	1:A:367:ARG:HH12	1.67	0.43
1:B:724:ASP:OD1	1:B:725:LYS:N	2.50	0.43
1:D:691:LEU:HA	1:D:691:LEU:HD23	1.78	0.43
1:A:482:GLU:O	1:A:483:SER:HB3	2.19	0.43
1:B:357:SER:HB2	1:B:358:HIS:HA	2.01	0.43
1:B:365:ILE:HG22	1:B:366:TYR:CD2	2.54	0.43
1:B:797:PHE:CD1	1:B:808:THR:HG22	2.53	0.43
1:B:832:ASN:O	1:B:836:SER:HB2	2.18	0.43
1:A:99:ARG:HB3	1:A:174:PHE:HB2	2.00	0.43
1:A:377:TRP:CD1	1:A:450:CYS:HG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:TRP:HA	1:A:560:ASN:HA	1.78	0.43
1:D:61:THR:OG1	1:D:166:PHE:HB3	2.19	0.43
1:D:455:ALA:HB2	1:D:478:VAL:HG22	2.00	0.43
1:A:225:VAL:O	1:A:241:GLN:HA	2.18	0.43
1:A:664:ASN:HB2	1:A:686:LEU:HD12	1.99	0.43
1:B:377:TRP:CZ3	1:B:509:PHE:CD1	3.06	0.43
1:B:572:SER:HB2	1:B:766:PRO:HG3	2.00	0.43
1:C:36:LYS:HD2	1:C:53:TRP:CE2	2.53	0.43
1:C:590:GLU:HG2	1:C:611:ASP:OD1	2.18	0.43
1:C:707:GLN:HB2	1:C:770:THR:HG21	2.01	0.43
1:C:735:MET:HG3	1:C:777:CYS:SG	2.58	0.43
1:C:786:VAL:HB	1:C:879:ARG:HG3	1.99	0.43
1:D:84:LYS:HD3	1:D:139:GLU:OE2	2.19	0.43
1:D:832:ASN:OD1	1:D:835:ASP:HB2	2.19	0.43
1:B:687:LEU:HA	1:B:687:LEU:HD23	1.79	0.43
1:C:618:ILE:CD1	1:C:687:LEU:HD23	2.49	0.43
1:C:780:LEU:HD22	1:C:875:VAL:HG21	2.01	0.43
1:B:152:LEU:O	1:B:154:GLU:N	2.52	0.43
1:C:283:ASP:HB2	1:C:290:TYR:CE2	2.54	0.43
1:C:598:ARG:NH1	1:C:653:ASN:HA	2.31	0.43
1:D:426:HIS:CE1	1:D:429:ALA:H	2.37	0.43
1:D:476:ASN:HD22	1:D:503:SER:HB2	1.83	0.43
1:D:735:MET:HE3	1:D:735:MET:HB3	1.84	0.43
1:A:115:LEU:HD12	1:A:116:LEU:N	2.34	0.43
1:A:425:TYR:HD1	1:A:461:PRO:HG3	1.84	0.43
1:A:536:GLN:O	1:A:540:ASN:ND2	2.45	0.43
1:B:846:THR:HB	1:C:28:SER:HB3	2.01	0.43
1:C:495:MET:HE2	1:C:495:MET:HB2	1.88	0.43
1:C:544:ILE:HG22	1:C:598:ARG:HH21	1.84	0.43
1:A:400:LEU:HD23	1:A:439:LEU:HG	2.00	0.42
1:A:500:CYS:HB3	1:A:508:ARG:HH21	1.84	0.42
1:B:741:ASN:CG	1:B:750:GLY:HA2	2.44	0.42
1:B:853:ASN:O	1:B:854:HIS:ND1	2.52	0.42
1:B:711:TYR:CD1	1:B:723:PRO:HD3	2.54	0.42
1:B:787:TYR:CE1	1:B:877:LYS:HB2	2.54	0.42
1:C:364:GLU:OE2	1:C:367:ARG:NH1	2.52	0.42
1:A:552:ASP:OD1	1:A:552:ASP:N	2.49	0.42
1:C:232:GLU:HB2	1:C:273:TYR:OH	2.19	0.42
1:C:480:VAL:HG21	1:C:496:PHE:CE2	2.55	0.42
1:C:858:GLU:OE1	1:C:860:LEU:HD21	2.19	0.42
1:D:185:THR:OG1	3:D:1005:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:PHE:HB3	1:B:684:MET:HE3	2.01	0.42
1:C:638:GLU:HB2	1:C:648:VAL:CG2	2.46	0.42
1:D:545:ASN:OD1	1:D:598:ARG:NH1	2.45	0.42
1:A:416:TRP:HB2	1:A:440:LYS:HD3	2.01	0.42
1:C:26:GLU:HG2	1:C:176:GLN:HB3	2.01	0.42
1:A:457:THR:HA	1:A:462:TYR:CD2	2.54	0.42
1:B:215:ASN:O	1:B:248:PRO:HA	2.20	0.42
1:C:183:PHE:CE2	1:C:213:LEU:HD11	2.54	0.42
1:C:598:ARG:NH1	1:C:653:ASN:C	2.77	0.42
1:C:873:LEU:HD12	1:C:873:LEU:HA	1.77	0.42
1:C:300:ARG:HE	1:C:411:PRO:HA	1.84	0.42
1:C:559:TRP:HA	1:C:560:ASN:HA	1.81	0.42
1:D:48:TRP:CG	1:D:49:ASN:N	2.87	0.42
1:D:59:PRO:HB3	1:D:170:TYR:C	2.44	0.42
1:C:250:ARG:HB3	1:C:252:TYR:CE2	2.55	0.42
1:C:675:ALA:C	1:C:676:LEU:HD23	2.45	0.42
1:C:705:LEU:HA	1:C:724:ASP:OD2	2.20	0.42
1:D:103:VAL:O	1:D:122:ALA:HA	2.20	0.42
1:D:326:ASP:HB3	1:D:332:THR:HG22	2.02	0.42
1:D:537:LEU:HG	1:D:541:ARG:HH11	1.84	0.42
1:D:619:CYS:HB3	1:D:686:LEU:HG	2.02	0.42
1:D:705:LEU:HD23	1:D:705:LEU:HA	1.84	0.42
1:B:207:MET:HE1	1:B:229:LEU:HD13	2.02	0.42
1:B:562:VAL:HG11	1:B:586:ARG:CZ	2.50	0.42
1:C:220:THR:HG23	1:C:247:ILE:HA	2.01	0.42
1:C:832:ASN:O	1:C:836:SER:HB2	2.20	0.42
1:C:839:GLU:HG3	1:C:840:GLN:HG3	2.02	0.42
1:D:454:HIS:CE1	1:D:456:PHE:HB2	2.55	0.42
1:D:456:PHE:N	1:D:456:PHE:CD2	2.88	0.42
1:B:348:GLU:O	1:B:596:GLN:NE2	2.52	0.42
1:D:527:ARG:NH1	3:D:1023:HOH:O	2.53	0.42
1:A:564:PHE:O	1:A:576:LEU:HD12	2.20	0.41
1:A:581:MET:CE	1:A:591:ILE:HG23	2.50	0.41
1:B:298:GLY:N	1:B:411:PRO:HG3	2.35	0.41
1:B:660:VAL:HB	1:B:662:PHE:CE2	2.55	0.41
1:C:53:TRP:CZ3	1:C:82:ARG:HD3	2.55	0.41
1:C:731:SER:OG	1:C:732:TRP:N	2.50	0.41
1:A:187:PRO:HG2	1:A:188:TYR:CE2	2.56	0.41
1:A:194:ARG:HD3	1:A:194:ARG:N	2.35	0.41
1:A:458:TRP:HZ2	1:A:486:GLN:HE21	1.68	0.41
1:B:111:LEU:HD23	1:B:133:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:THR:HB	1:B:534:GLU:OE1	2.21	0.41
1:C:109:VAL:HG22	1:C:144:VAL:HG13	2.01	0.41
1:B:63:ASN:HA	1:B:66:ASP:HB2	2.02	0.41
1:C:259:GLY:O	1:C:261:ILE:HG13	2.20	0.41
1:D:92:ARG:NH2	1:D:136:VAL:O	2.53	0.41
1:B:32:SER:O	1:B:32:SER:OG	2.31	0.41
1:A:346:LEU:HD12	1:A:349:MET:HE2	2.03	0.41
1:A:540:ASN:O	1:A:544:ILE:HG12	2.21	0.41
1:B:760:LYS:HB2	1:B:841:THR:HG23	2.02	0.41
1:D:106:LYS:HG3	1:D:120:LEU:CD2	2.51	0.41
1:D:220:THR:CG2	1:D:248:PRO:HD3	2.51	0.41
1:D:353:PHE:HE2	1:D:557:SER:OG	2.02	0.41
1:A:876:LYS:HB2	1:A:876:LYS:HE3	1.78	0.41
1:C:154:GLU:HG3	1:C:389:ASN:ND2	2.34	0.41
1:C:373:GLY:O	1:C:374:LEU:HG	2.20	0.41
1:D:53:TRP:CZ3	1:D:82:ARG:HD3	2.56	0.41
1:D:355:ARG:HH12	1:D:512:GLU:HG3	1.86	0.41
1:D:560:ASN:O	1:D:580:GLY:HA2	2.21	0.41
1:A:691:LEU:HD13	1:A:782:VAL:HG12	2.03	0.41
1:A:694:SER:OG	1:A:695:ASP:N	2.53	0.41
1:C:581:MET:HB3	1:C:581:MET:HE3	1.72	0.41
1:D:116:LEU:CD1	1:D:130:ILE:HG22	2.50	0.41
1:D:301:TRP:CE2	1:D:312:ASN:HA	2.56	0.41
1:A:434:ARG:HG2	1:A:472:ILE:HD13	2.02	0.41
1:B:251:LYS:HB3	1:B:251:LYS:HE2	1.70	0.41
1:B:451:VAL:HG12	1:B:476:ASN:HA	2.03	0.41
1:C:380:ILE:HG13	1:C:418:ALA:HA	2.02	0.41
1:D:121:GLY:H	1:D:156:LEU:HD21	1.86	0.41
1:D:233:MET:HE3	1:D:233:MET:HB3	1.97	0.41
1:B:591:ILE:HD12	1:B:591:ILE:HA	1.80	0.41
1:C:33:TRP:CD2	1:C:83:LYS:HB2	2.55	0.41
1:C:530:ASP:CG	1:C:532:THR:HG1	2.26	0.41
1:C:705:LEU:HD23	1:C:724:ASP:OD2	2.21	0.41
1:C:707:GLN:CD	1:C:710:CYS:HB2	2.46	0.41
1:C:727:TYR:HB2	1:C:733:GLY:C	2.46	0.41
1:C:300:ARG:HD3	1:C:300:ARG:N	2.35	0.41
1:D:66:ASP:O	3:D:1004:HOH:O	2.20	0.41
1:D:323:ARG:CZ	1:D:365:ILE:HD11	2.51	0.41
1:A:794:THR:C	1:A:833:LEU:HD13	2.46	0.40
1:C:157:PRO:HG2	1:C:399:MET:HE1	2.03	0.40
1:C:466:SER:OG	1:C:467:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:TYR:HD1	1:D:502:TYR:CE2	2.38	0.40
1:D:544:ILE:HD12	1:D:556:TYR:HE2	1.87	0.40
1:A:458:TRP:HD1	1:A:459:GLU:OE1	2.03	0.40
1:B:526:PRO:HG3	1:B:534:GLU:HB3	2.03	0.40
1:B:700:GLY:HA2	1:B:875:VAL:O	2.20	0.40
1:C:302:PHE:CZ	1:C:447:ARG:HA	2.56	0.40
1:D:96:ILE:H	1:D:131:THR:HG23	1.86	0.40
1:D:213:LEU:HD21	1:D:281:VAL:HG21	2.04	0.40
1:A:712:PHE:CE1	1:A:766:PRO:HG2	2.56	0.40
1:B:354:VAL:HG11	1:B:369:CYS:SG	2.61	0.40
1:B:702:CYS:HB3	1:B:721:TRP:CD2	2.56	0.40
1:C:514:GLY:HA3	1:C:559:TRP:O	2.21	0.40
1:D:228:PHE:CD1	1:D:228:PHE:N	2.89	0.40
1:D:461:PRO:HB3	1:D:469:MET:HE2	2.04	0.40
1:D:695:ASP:OD1	1:D:695:ASP:N	2.48	0.40
1:A:525:THR:O	1:A:525:THR:OG1	2.31	0.40
1:B:190:ALA:HB2	1:B:405:LEU:HB3	2.03	0.40
1:B:304:VAL:HG23	1:B:304:VAL:O	2.20	0.40
1:B:628:ILE:O	1:B:657:VAL:HA	2.22	0.40
1:D:212:PHE:HE1	1:D:253:PRO:HB3	1.86	0.40
1:D:213:LEU:CD1	1:D:254:ILE:HD11	2.51	0.40
1:D:762:THR:HG21	1:D:768:PHE:CD2	2.56	0.40
1:D:876:LYS:HB2	1:D:876:LYS:HE3	1.69	0.40
1:A:507:PRO:HA	1:A:508:ARG:NH1	2.37	0.40
1:A:668:LEU:HD21	1:A:679:ARG:NH2	2.36	0.40
1:B:488:ASP:O	1:B:490:ALA:N	2.54	0.40
1:D:194:ARG:HB3	1:D:408:TYR:CE2	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLU:OE1	1:D:852:ARG:NH1[1_565]	2.06	0.14
1:A:855:GLU:OE2	1:D:22:SER:OG[1_565]	2.11	0.09

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	858/879 (98%)	783 (91%)	69 (8%)	6 (1%)	18	48
1	B	858/879 (98%)	786 (92%)	63 (7%)	9 (1%)	12	39
1	C	858/879 (98%)	780 (91%)	69 (8%)	9 (1%)	12	39
1	D	858/879 (98%)	771 (90%)	79 (9%)	8 (1%)	14	41
All	All	3432/3516 (98%)	3120 (91%)	280 (8%)	32 (1%)	14	41

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	830	SER
1	B	830	SER
1	C	104	ALA
1	C	105	SER
1	B	32	SER
1	B	219	ASP
1	B	823	ASN
1	C	830	SER
1	A	32	SER
1	A	66	ASP
1	A	709	HIS
1	B	489	SER
1	C	49	ASN
1	C	356	ILE
1	C	586	ARG
1	D	138	LYS
1	D	424	ASP
1	D	571	ASP
1	B	66	ASP
1	B	571	ASP
1	C	32	SER
1	C	571	ASP

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Mol	Chain	Res	Type
1	D	272	PRO
1	D	388	LYS
1	D	553	TYR
1	A	162	ASP
1	B	492	ILE
1	B	674	GLY
1	C	285	LYS
1	D	418	ALA
1	A	544	ILE
1	D	356	ILE

5.3.2 Protein sidechains [i](#)

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	750/775 (97%)	748 (100%)	2 (0%)	86	96
1	B	752/775 (97%)	750 (100%)	2 (0%)	86	96
1	C	752/775 (97%)	752 (100%)	0	100	100
1	D	739/775 (95%)	738 (100%)	1 (0%)	88	97
All	All	2993/3100 (96%)	2988 (100%)	5 (0%)	87	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	650	GLU
1	B	195	ILE
1	B	209	ILE
1	D	155	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	GLN

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Mol	Chain	Res	Type
1	A	389	ASN
1	A	707	GLN
1	A	718	GLN
1	B	196	GLN
1	B	265	HIS
1	B	389	ASN
1	B	486	GLN
1	B	634	GLN
1	B	664	ASN
1	B	709	HIS
1	B	804	ASN
1	B	867	GLN
1	C	176	GLN
1	C	389	ASN
1	C	716	GLN
1	C	853	ASN
1	D	196	GLN
1	D	215	ASN
1	D	339	ASN
1	D	540	ASN
1	D	718	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	860/879 (97%)	-0.34	0	100 100	11, 27, 44, 65	0
1	B	860/879 (97%)	-0.43	0	100 100	11, 23, 41, 57	0
1	C	860/879 (97%)	-0.37	1 (0%)	92 90	14, 27, 48, 61	0
1	D	860/879 (97%)	-0.08	5 (0%)	85 81	15, 33, 59, 77	0
All	All	3440/3516 (97%)	-0.30	6 (0%)	91 89	11, 27, 51, 77	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	66	ASP	3.1
1	D	203	SER	2.8
1	D	313	GLY	2.3
1	D	206	SER	2.2
1	D	207	MET	2.2
1	D	275	TYR	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(Å ²)	Q<0.9
2	NA	A	901	1/1	0.93	0.07	27,27,27,27	0
2	NA	C	901	1/1	0.97	0.05	21,21,21,21	0
2	NA	D	901	1/1	0.97	0.04	17,17,17,17	0
2	NA	B	901	1/1	1.00	0.05	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.