



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:29 AM UTC

PDB ID : 3CU1 / pdb_00003cu1
Title : Crystal Structure of 2:2:2 FGFR2D2:FGF1:SOS complex
Authors : Guo, F.; Dakshinamurthy, R.; Thallapuranam, S.K.K.; Sakon, J.
Deposited on : 2008-04-15
Resolution : 2.60 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
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

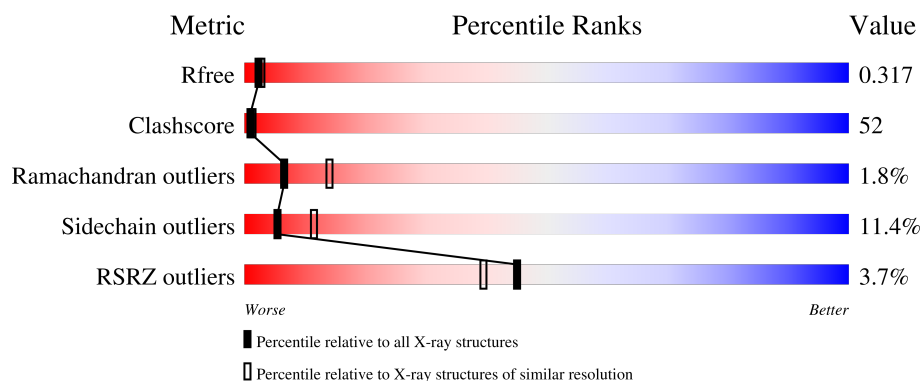
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	100	4% 19% 42% 35% .
1	C	100	4% 26% 40% 33% .
2	B	131	2% 25% 45% 22% 5% .
2	D	131	5% 21% 39% 29% 11%
3	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GU4	F	1	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4183 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.

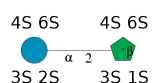
- Molecule 1 is a protein called Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	3	0
			832	524	157	145	6			
1	C	100	Total	C	N	O	S	0	2	0
			825	520	154	145	6			

- Molecule 2 is a protein called Heparin-binding growth factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	128	Total	C	N	O	S	0	0	0
			1022	646	179	193	4			
2	D	131	Total	C	N	O	S	0	0	0
			1051	665	184	198	4			

- Molecule 3 is an oligosaccharide called 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	O	S	0	0	0
			55	12	35	8			
3	F	2	Total	C	O	S	0	0	0
			55	12	35	8			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	80	Total	O	0	0
			80	80		

Continued on next page...

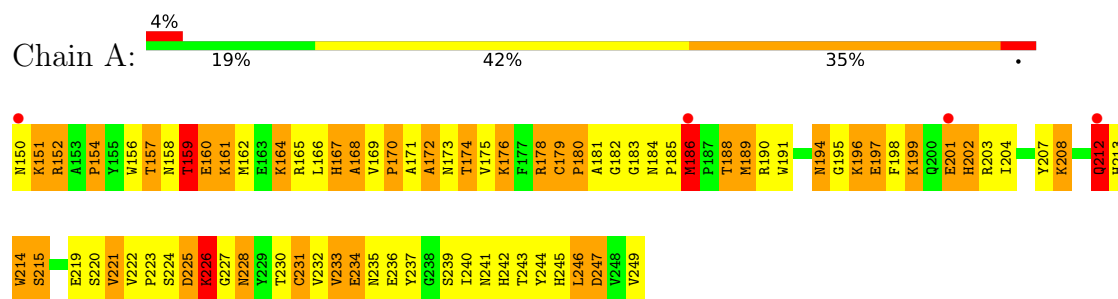
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	68	Total 68	O 68	0	0
4	C	98	Total 98	O 98	0	0
4	D	97	Total 97	O 97	0	0

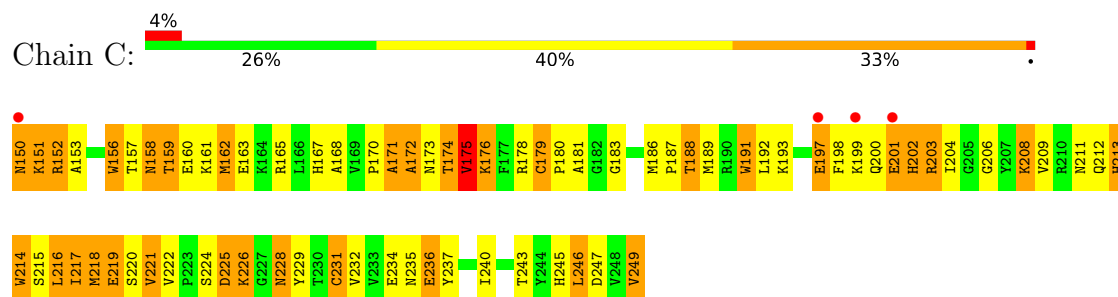
3 Residue-property plots

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.

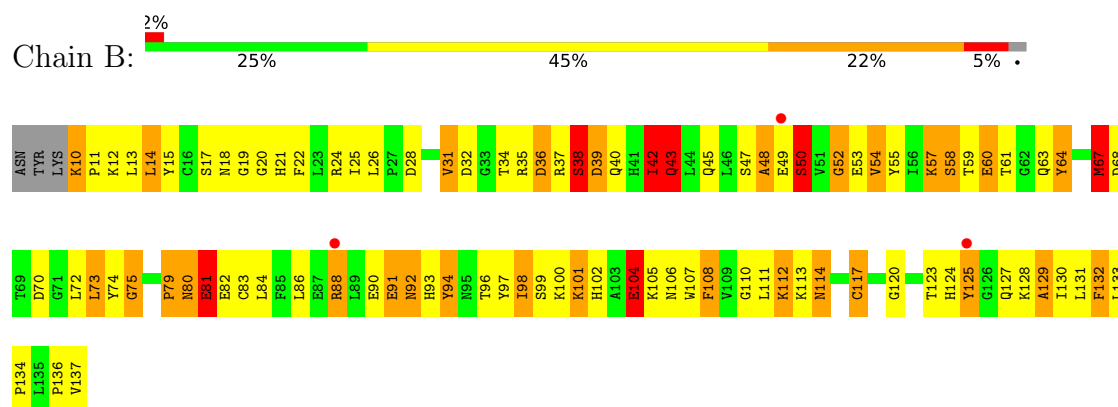
• Molecule 1: Fibroblast growth factor receptor 2



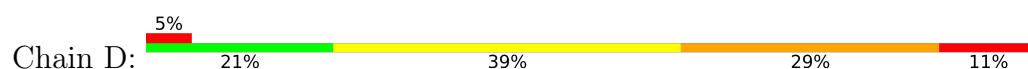
• Molecule 1: Fibroblast growth factor receptor 2

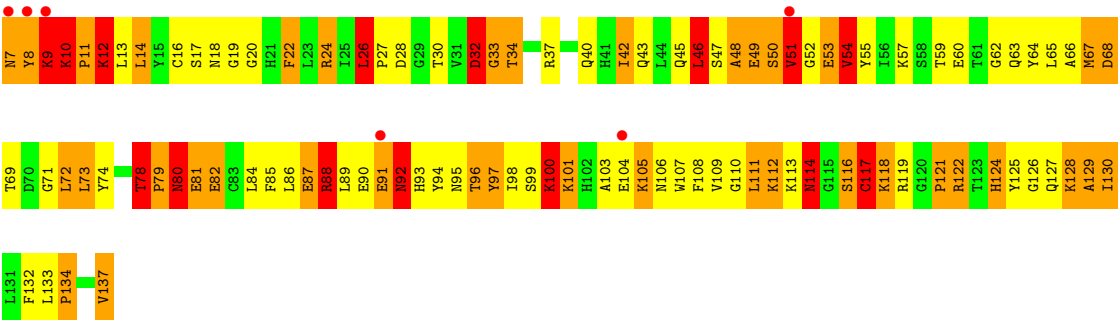


• Molecule 2: Heparin-binding growth factor 1



• Molecule 2: Heparin-binding growth factor 1





● Molecule 3: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain E: 100%

GU41
YYJ2

● Molecule 3: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain F: 100%

GU41
YYJ2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.93Å 110.38Å 74.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.95 – 2.60 42.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.0 (42.95-2.60) 90.0 (42.95-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.24 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.277 0.261 , 0.317	Depositor DCC
R_{free} test set	1044 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.3	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	4183	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% 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: GU4, YYJ

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	3.07	105/868 (12.1%)	1.80	21/1173 (1.8%)
1	C	3.13	87/857 (10.2%)	1.83	23/1159 (2.0%)
2	B	2.55	66/1045 (6.3%)	1.74	26/1410 (1.8%)
2	D	2.86	93/1075 (8.7%)	1.88	37/1450 (2.6%)
All	All	2.89	351/3845 (9.1%)	1.81	107/5192 (2.1%)

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
2	D	2	0

All (351) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	171	ALA	CA-CB	-12.61	1.32	1.53
1	C	158	ASN	CA-CB	-12.01	1.44	1.53
1	A	247	ASP	CA-C	11.71	1.66	1.52
2	B	91	GLU	C-O	-10.70	1.10	1.24
1	A	242	HIS	CA-C	-10.64	1.39	1.52
1	C	156	TRP	C-O	-10.61	1.10	1.23
1	C	204	ILE	CA-C	10.50	1.64	1.52
1	A	232	VAL	CA-CB	-10.49	1.41	1.54
2	B	98	ILE	CA-CB	-10.26	1.41	1.54
1	C	243	THR	C-O	-10.23	1.11	1.24
1	A	186	MET	SD-CE	10.16	2.04	1.79
2	D	118	LYS	CE-NZ	10.01	1.79	1.49
1	C	225	ASP	C-O	-10.01	1.11	1.24
1	A	228	ASN	CA-C	-10.01	1.40	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	170	PRO	CA-C	-9.90	1.40	1.52
1	C	151	LYS	CA-C	9.80	1.66	1.52
1	A	167	HIS	C-O	9.54	1.35	1.24
1	C	162	MET	N-CA	-9.42	1.32	1.46
2	B	113	LYS	C-O	-9.42	1.11	1.24
1	C	208	LYS	CB-CG	-9.42	1.24	1.52
2	D	132	PHE	CA-C	-9.37	1.41	1.52
1	C	186	MET	C-O	-9.23	1.12	1.24
2	B	14	LEU	CG-CD1	-9.19	1.22	1.52
1	C	222	VAL	CA-C	9.17	1.62	1.52
2	D	73	LEU	C-O	8.99	1.35	1.23
2	D	26	LEU	CG-CD2	8.97	1.82	1.52
2	D	65	LEU	CA-CB	-8.94	1.39	1.53
1	C	167	HIS	N-CA	-8.91	1.34	1.46
2	D	91	GLU	N-CA	-8.84	1.34	1.46
1	C	218	MET	CB-CG	-8.84	1.25	1.52
2	B	64	TYR	C-O	8.81	1.34	1.23
2	D	112	LYS	CA-C	8.75	1.64	1.53
1	A	202	HIS	CA-C	8.73	1.65	1.52
2	D	48	ALA	CA-C	8.70	1.64	1.52
1	C	197	GLU	CG-CD	8.63	1.73	1.52
1	A	176	LYS	C-O	-8.56	1.14	1.24
2	D	82	GLU	C-O	8.55	1.35	1.24
1	A	222	VAL	N-CA	8.53	1.57	1.46
2	D	111	LEU	C-O	-8.44	1.14	1.24
1	C	183	GLY	CA-C	8.43	1.60	1.51
2	D	101	LYS	CA-C	8.40	1.63	1.52
1	A	228	ASN	C-O	-8.38	1.13	1.24
2	D	134	PRO	CA-C	8.34	1.60	1.52
2	D	85	PHE	CA-C	-8.34	1.42	1.52
2	D	130	ILE	CA-CB	-8.34	1.42	1.54
2	D	128	LYS	CD-CE	8.32	1.77	1.52
1	C	198	PHE	CA-C	8.30	1.63	1.53
2	D	117	CYS	CA-CB	-8.23	1.40	1.53
1	A	168	ALA	CA-CB	-8.23	1.42	1.53
2	D	20	GLY	C-O	8.16	1.35	1.24
2	D	112	LYS	CD-CE	-8.15	1.28	1.52
1	C	176	LYS	C-O	-8.07	1.14	1.24
2	D	121	PRO	C-O	-8.07	1.14	1.24
1	A	166	LEU	CA-C	-8.04	1.43	1.52
1	A	171	ALA	N-CA	7.94	1.56	1.45
1	C	232	VAL	CA-CB	-7.94	1.44	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	204	ILE	CA-CB	-7.87	1.45	1.54
2	B	133	LEU	C-N	-7.86	1.27	1.33
1	A	181	ALA	CA-CB	-7.85	1.40	1.53
2	D	84	LEU	C-O	-7.85	1.14	1.23
1	A	196	LYS	CE-NZ	7.83	1.72	1.49
1	C	247	ASP	CA-C	7.81	1.61	1.52
2	D	71	GLY	CA-C	-7.74	1.40	1.51
1	C	211	ASN	C-O	-7.72	1.15	1.24
2	B	43	GLN	CA-CB	-7.71	1.42	1.53
1	C	204	ILE	N-CA	-7.70	1.36	1.46
1	C	175	VAL	C-O	7.69	1.31	1.24
1	A	162	MET	N-CA	-7.67	1.35	1.46
1	C	228	ASN	CA-C	-7.66	1.43	1.52
2	D	122	ARG	NE-CZ	7.62	1.41	1.33
2	D	122	ARG	CD-NE	7.58	1.56	1.46
1	A	174	THR	CA-CB	-7.58	1.40	1.53
1	C	202	HIS	CA-CB	7.57	1.65	1.53
2	B	131	LEU	C-O	7.54	1.33	1.24
2	D	81	GLU	CB-CG	-7.54	1.29	1.52
2	D	91	GLU	C-O	-7.53	1.14	1.24
1	C	217	ILE	CA-CB	-7.51	1.44	1.54
2	D	66	ALA	C-O	7.49	1.32	1.23
1	C	193	LYS	C-O	-7.47	1.15	1.24
1	C	197	GLU	CB-CG	7.42	1.74	1.52
2	D	17	SER	C-O	-7.40	1.14	1.24
2	D	14	LEU	C-O	7.38	1.33	1.24
2	D	64	TYR	C-O	7.30	1.32	1.23
2	D	26	LEU	CA-C	-7.29	1.43	1.52
1	A	170	PRO	C-O	-7.28	1.16	1.23
1	C	201	GLU	C-O	-7.27	1.14	1.24
2	D	68	ASP	CB-CG	-7.24	1.33	1.52
1	C	174	THR	CA-CB	-7.23	1.41	1.53
1	A	225	ASP	CG-OD1	7.22	1.39	1.25
2	D	34	THR	CA-C	-7.20	1.43	1.52
2	B	57	LYS	CE-NZ	7.19	1.71	1.49
2	B	82	GLU	C-O	7.19	1.33	1.24
1	C	152	ARG	N-CA	7.18	1.54	1.46
1	A	198	PHE	CA-C	7.18	1.62	1.53
2	D	117	CYS	CB-SG	-7.18	1.57	1.81
1	A	152	ARG	CA-CB	-7.16	1.41	1.53
1	C	215	SER	N-CA	-7.15	1.36	1.45
1	C	175	VAL	CB-CG2	-7.15	1.28	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	42	ILE	CA-CB	7.08	1.63	1.54
1	C	232	VAL	C-O	-7.00	1.16	1.24
2	B	31	VAL	C-O	-6.98	1.17	1.24
1	A	227	GLY	CA-C	-6.96	1.45	1.52
1	C	246	LEU	CG-CD1	-6.96	1.29	1.52
2	B	55	TYR	N-CA	-6.92	1.37	1.46
1	C	218	MET	C-O	-6.92	1.16	1.24
1	C	150	ASN	CB-CG	-6.90	1.34	1.52
1	C	186	MET	SD-CE	6.88	1.96	1.79
1	A	188	THR	C-O	-6.85	1.14	1.23
2	B	123	THR	N-CA	6.85	1.54	1.45
2	D	87	GLU	C-O	-6.85	1.15	1.24
2	D	95	ASN	N-CA	-6.83	1.37	1.45
2	D	99	SER	CA-C	6.81	1.61	1.52
1	A	179	CYS	CA-CB	-6.80	1.42	1.53
2	D	100	LYS	N-CA	-6.80	1.38	1.46
2	B	134	PRO	C-O	6.79	1.30	1.23
2	B	32	ASP	C-O	-6.78	1.19	1.24
1	C	157	THR	N-CA	-6.77	1.36	1.46
2	B	36	ASP	N-CA	6.77	1.54	1.46
1	A	189	MET	CG-SD	6.75	1.97	1.80
2	D	81	GLU	CA-CB	-6.70	1.42	1.53
1	A	152	ARG	CB-CG	-6.67	1.32	1.52
1	C	243	THR	CA-C	-6.66	1.44	1.52
1	A	178[A]	ARG	N-CA	6.66	1.54	1.45
1	A	178[B]	ARG	N-CA	6.66	1.54	1.45
2	D	97	TYR	CA-C	-6.65	1.44	1.52
1	A	247	ASP	CG-OD2	6.64	1.38	1.25
1	C	222	VAL	CA-CB	-6.63	1.45	1.54
2	D	72	LEU	C-O	6.63	1.31	1.24
1	C	173	ASN	CG-OD1	-6.62	1.10	1.23
2	B	38	SER	CA-C	6.59	1.61	1.52
1	A	221	VAL	N-CA	-6.59	1.38	1.46
2	D	104	GLU	CG-CD	6.57	1.68	1.52
2	D	133	LEU	C-N	-6.57	1.28	1.33
1	C	203	ARG	CA-C	-6.57	1.44	1.52
1	C	201	GLU	CB-CG	6.55	1.72	1.52
1	A	176	LYS	CA-C	-6.55	1.44	1.52
2	B	31	VAL	CA-C	6.55	1.60	1.52
2	B	112	LYS	CE-NZ	6.54	1.69	1.49
2	B	83	CYS	CA-C	-6.53	1.44	1.52
2	B	129	ALA	CA-C	6.52	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	183	GLY	N-CA	6.52	1.52	1.45
1	A	190	ARG	CB-CG	-6.52	1.32	1.52
1	A	165	ARG	CA-C	-6.49	1.43	1.52
1	A	241	ASN	N-CA	6.48	1.54	1.45
1	A	221	VAL	CB-CG2	-6.48	1.31	1.52
2	D	17	SER	CA-C	6.46	1.61	1.52
1	C	191	TRP	CE3-CZ3	6.45	1.57	1.38
1	A	233	VAL	CA-CB	-6.44	1.46	1.54
2	B	48	ALA	CA-CB	-6.44	1.42	1.53
2	D	97	TYR	N-CA	-6.43	1.38	1.46
2	D	11	PRO	N-CA	6.43	1.55	1.47
2	D	9	LYS	N-CA	6.42	1.54	1.46
1	A	159	THR	CA-C	6.38	1.61	1.52
2	D	124	HIS	CA-C	-6.36	1.44	1.52
1	C	203	ARG	CG-CD	6.34	1.71	1.52
1	A	241	ASN	CA-CB	-6.34	1.42	1.54
1	A	233	VAL	C-O	6.33	1.31	1.24
1	C	214	TRP	C-O	-6.33	1.15	1.23
1	A	150	ASN	CB-CG	-6.31	1.36	1.52
1	A	203	ARG	C-O	-6.29	1.15	1.23
2	D	87	GLU	CD-OE1	6.28	1.37	1.25
2	D	14	LEU	CA-CB	-6.28	1.45	1.53
2	B	25	ILE	C-O	-6.28	1.15	1.23
2	D	116	SER	C-O	-6.25	1.15	1.23
2	B	54	VAL	N-CA	-6.25	1.39	1.46
2	D	54	VAL	N-CA	-6.24	1.39	1.46
2	B	108	PHE	CA-C	-6.24	1.44	1.53
1	A	201	GLU	C-O	-6.23	1.15	1.24
2	D	128	LYS	CE-NZ	6.21	1.68	1.49
1	A	234	GLU	N-CA	-6.21	1.37	1.45
2	D	32	ASP	C-O	-6.21	1.18	1.24
1	A	225	ASP	C-O	-6.21	1.15	1.24
2	B	20	GLY	CA-C	6.20	1.59	1.51
1	C	172	ALA	N-CA	-6.20	1.34	1.46
1	A	160	GLU	CD-OE2	6.19	1.37	1.25
1	A	161	LYS	N-CA	6.17	1.53	1.46
1	A	175	VAL	CA-C	-6.17	1.45	1.52
2	B	21	HIS	CA-C	-6.15	1.44	1.52
1	A	212[A]	GLN	CA-C	6.12	1.61	1.52
1	A	212[B]	GLN	CA-C	6.12	1.61	1.52
2	D	7	ASN	CB-CG	6.11	1.67	1.52
2	B	92	ASN	C-O	-6.10	1.14	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	THR	CA-CB	-6.09	1.44	1.53
2	D	74	TYR	C-N	6.09	1.39	1.33
2	D	20	GLY	C-N	6.08	1.42	1.33
2	B	111	LEU	C-O	-6.08	1.17	1.23
1	C	176	LYS	CG-CD	6.08	1.70	1.52
1	C	209	VAL	C-O	-6.07	1.17	1.24
1	A	161	LYS	CB-CG	6.07	1.70	1.52
1	A	221	VAL	C-O	6.06	1.30	1.24
1	A	227	GLY	N-CA	-6.05	1.39	1.45
2	B	60	GLU	N-CA	-6.05	1.37	1.46
1	C	151	LYS	C-O	-6.03	1.16	1.24
1	C	203	ARG	N-CA	6.03	1.53	1.46
1	C	203	ARG	CB-CG	-6.03	1.34	1.52
1	C	201	GLU	CG-CD	6.01	1.67	1.52
2	D	10	LYS	CA-CB	6.00	1.62	1.53
2	D	16	CYS	C-O	-5.99	1.16	1.24
1	A	242	HIS	C-O	-5.99	1.16	1.23
1	A	160	GLU	CA-CB	5.99	1.63	1.53
2	B	120	GLY	N-CA	5.97	1.52	1.44
2	B	48	ALA	N-CA	5.97	1.53	1.46
1	C	198	PHE	N-CA	-5.96	1.38	1.46
2	D	134	PRO	C-O	-5.96	1.18	1.23
1	A	169	VAL	CB-CG1	-5.95	1.32	1.52
2	D	88	ARG	NE-CZ	5.95	1.39	1.33
2	D	82	GLU	N-CA	-5.95	1.38	1.46
1	C	163	GLU	CD-OE1	5.93	1.36	1.25
2	B	68	ASP	C-O	-5.93	1.16	1.23
2	B	110	GLY	CA-C	5.92	1.57	1.52
1	A	172	ALA	N-CA	-5.91	1.35	1.46
2	D	46	LEU	C-O	-5.90	1.16	1.23
1	C	168	ALA	CA-CB	5.89	1.61	1.53
1	C	231	CYS	N-CA	-5.89	1.38	1.46
1	A	156	TRP	CZ3-CH2	-5.88	1.25	1.40
1	C	228	ASN	CA-CB	-5.87	1.45	1.53
1	C	211	ASN	N-CA	5.86	1.53	1.46
2	D	78	THR	CA-CB	5.86	1.61	1.53
1	A	168	ALA	C-O	-5.84	1.17	1.24
1	A	228	ASN	CA-CB	-5.83	1.44	1.53
1	A	219	GLU	CG-CD	5.82	1.66	1.52
2	B	50	SER	CA-C	5.82	1.61	1.53
2	B	73	LEU	CA-CB	-5.81	1.44	1.53
2	D	24	ARG	CA-CB	-5.80	1.43	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	96	THR	N-CA	5.79	1.53	1.45
1	A	190	ARG	CA-CB	-5.78	1.43	1.53
2	D	106	ASN	CA-C	-5.77	1.45	1.53
2	D	95	ASN	C-O	5.77	1.30	1.23
1	A	243	THR	CA-C	-5.76	1.45	1.52
1	A	204	ILE	C-O	5.75	1.29	1.24
2	D	74	TYR	C-O	5.74	1.30	1.23
1	A	152	ARG	CZ-NH2	5.72	1.40	1.33
1	C	176	LYS	CD-CE	5.72	1.69	1.52
1	A	186	MET	N-CA	5.71	1.53	1.45
1	C	197	GLU	CA-CB	5.71	1.62	1.53
1	C	191	TRP	N-CA	5.71	1.53	1.46
1	A	198	PHE	N-CA	-5.71	1.38	1.46
1	A	244	TYR	N-CA	5.70	1.52	1.45
1	A	194	ASN	N-CA	5.69	1.55	1.46
1	C	213	HIS	CA-C	5.69	1.60	1.52
1	C	170	PRO	N-CA	5.67	1.53	1.46
1	C	192	LEU	C-O	5.67	1.30	1.23
1	A	185	PRO	CG-CD	-5.67	1.36	1.51
1	A	183	GLY	N-CA	5.67	1.51	1.45
1	A	195	GLY	CA-C	5.66	1.59	1.51
1	A	160	GLU	CG-CD	5.66	1.66	1.52
1	A	208	LYS	CD-CE	5.65	1.69	1.52
2	D	88	ARG	CG-CD	5.65	1.69	1.52
1	A	215	SER	C-O	-5.64	1.16	1.23
1	C	228	ASN	C-O	-5.63	1.17	1.24
1	C	162	MET	C-O	-5.63	1.15	1.24
1	A	196	LYS	CD-CE	5.63	1.69	1.52
1	A	180	PRO	C-O	-5.62	1.16	1.23
2	D	88	ARG	CD-NE	5.62	1.54	1.46
2	D	128	LYS	CB-CG	5.61	1.69	1.52
2	D	14	LEU	N-CA	-5.60	1.39	1.46
2	B	73	LEU	C-O	5.60	1.30	1.23
2	B	132	PHE	CE1-CZ	5.58	1.55	1.38
2	B	94	TYR	CB-CG	-5.56	1.39	1.51
1	A	175	VAL	CA-CB	5.55	1.64	1.55
2	B	125	TYR	CD1-CE1	5.54	1.55	1.38
1	A	164	LYS	C-O	5.52	1.30	1.23
1	A	174	THR	C-O	-5.52	1.17	1.23
2	D	54	VAL	CA-C	-5.52	1.46	1.52
2	B	97	TYR	CA-C	-5.51	1.45	1.52
1	C	249	VAL	N-CA	-5.50	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	ALA	CA-CB	5.49	1.62	1.53
1	A	151	LYS	CA-C	5.49	1.59	1.52
2	B	45	GLN	C-O	-5.49	1.17	1.24
2	B	75	GLY	C-O	5.49	1.31	1.23
1	A	201	GLU	N-CA	-5.49	1.38	1.46
2	D	53	GLU	N-CA	-5.49	1.40	1.46
1	C	224	SER	C-O	-5.49	1.17	1.24
1	C	179	CYS	N-CA	5.48	1.53	1.46
1	C	226	LYS	CG-CD	5.47	1.68	1.52
1	A	234	GLU	CD-OE1	5.46	1.35	1.25
1	C	181	ALA	CA-CB	-5.46	1.44	1.53
2	D	19	GLY	C-N	5.45	1.40	1.33
2	B	92	ASN	CA-C	-5.45	1.45	1.52
1	C	153	ALA	C-O	-5.45	1.17	1.24
1	A	231	CYS	N-CA	-5.44	1.39	1.46
2	D	113	LYS	C-O	-5.43	1.17	1.24
1	A	182	GLY	CA-C	5.42	1.57	1.52
1	C	208	LYS	C-O	-5.42	1.17	1.24
1	C	213	HIS	C-O	-5.41	1.17	1.24
2	D	54	VAL	C-O	-5.40	1.18	1.23
2	B	28	ASP	N-CA	5.40	1.53	1.46
2	B	130	ILE	C-O	5.39	1.32	1.23
2	D	12	LYS	C-N	5.39	1.40	1.33
2	D	68	ASP	CA-C	-5.39	1.45	1.53
2	B	98	ILE	N-CA	-5.38	1.40	1.46
1	C	165	ARG	CZ-NH2	5.38	1.40	1.33
2	B	70	ASP	CA-C	5.37	1.60	1.52
1	C	208	LYS	CA-C	-5.37	1.46	1.52
2	D	126	GLY	C-O	-5.37	1.17	1.24
2	B	134	PRO	CA-CB	5.37	1.60	1.53
1	A	164	LYS	CA-C	-5.36	1.45	1.52
2	D	65	LEU	CA-C	5.36	1.59	1.52
1	C	236	GLU	CD-OE1	5.35	1.35	1.25
2	D	53	GLU	CA-C	-5.35	1.46	1.52
2	D	69	THR	N-CA	-5.34	1.39	1.46
2	B	24	ARG	CB-CG	-5.34	1.36	1.52
1	A	154	PRO	C-O	5.33	1.29	1.23
2	B	81	GLU	N-CA	5.33	1.53	1.46
2	D	117	CYS	CA-C	-5.32	1.45	1.52
1	A	235	ASN	CB-CG	-5.31	1.38	1.52
1	C	188	THR	C-O	-5.29	1.16	1.23
2	B	104	GLU	CD-OE1	5.28	1.35	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	ARG	CG-CD	-5.26	1.36	1.52
2	B	17	SER	C-O	-5.25	1.17	1.24
1	C	191	TRP	C-O	-5.24	1.17	1.24
1	A	232	VAL	C-O	-5.23	1.18	1.24
1	A	159	THR	CA-CB	-5.22	1.45	1.53
2	D	87	GLU	CD-OE2	5.21	1.35	1.25
1	A	161	LYS	CD-CE	5.20	1.68	1.52
2	B	10	LYS	CD-CE	5.19	1.68	1.52
2	D	32	ASP	CB-CG	-5.18	1.39	1.52
1	A	240	ILE	CA-C	5.18	1.59	1.52
1	A	150	ASN	CA-CB	-5.17	1.43	1.53
2	B	104	GLU	CG-CD	5.16	1.65	1.52
2	D	67	MET	N-CA	-5.16	1.39	1.46
2	B	22	PHE	CB-CG	-5.16	1.38	1.50
1	C	219	GLU	N-CA	-5.16	1.39	1.45
2	B	127	GLN	CA-C	-5.15	1.45	1.53
1	A	224	SER	CA-CB	-5.14	1.44	1.53
1	A	161	LYS	CE-NZ	5.14	1.64	1.49
1	A	197	GLU	CB-CG	-5.12	1.37	1.52
1	A	182	GLY	C-O	5.12	1.30	1.23
2	B	60	GLU	CB-CG	-5.09	1.37	1.52
2	B	22	PHE	CA-CB	-5.09	1.45	1.53
1	C	209	VAL	CA-C	5.08	1.58	1.52
1	C	231	CYS	C-O	-5.07	1.17	1.24
2	D	33	GLY	CA-C	-5.07	1.47	1.52
1	A	174	THR	CB-CG2	5.07	1.69	1.52
2	B	10	LYS	CA-C	5.06	1.63	1.52
2	B	14	LEU	N-CA	-5.05	1.40	1.46
1	A	242	HIS	N-CA	5.05	1.52	1.45
2	D	48	ALA	N-CA	5.05	1.52	1.46
1	A	219	GLU	CD-OE1	5.05	1.34	1.25
2	D	54	VAL	C-N	-5.05	1.26	1.33
2	B	75	GLY	CA-C	5.04	1.55	1.52
1	C	165	ARG	CB-CG	-5.04	1.37	1.52
1	A	226	LYS	N-CA	5.04	1.52	1.46
2	B	67	MET	CB-CG	-5.04	1.37	1.52
2	B	17	SER	CA-CB	-5.04	1.44	1.53
2	B	60	GLU	CA-CB	-5.03	1.45	1.53
2	B	22	PHE	CA-C	-5.03	1.46	1.52
2	D	109	VAL	CA-CB	5.03	1.59	1.54
1	A	189	MET	CA-C	5.02	1.58	1.52
1	A	184	ASN	CA-CB	-5.01	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	124	HIS	CB-CG	-5.00	1.43	1.50

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	91	GLU	N-CA-C	15.05	131.90	112.34
2	B	92	ASN	N-CA-C	13.81	130.84	113.43
2	D	91	GLU	CA-C-N	12.23	143.71	121.70
2	D	91	GLU	C-N-CA	12.23	143.71	121.70
1	A	186	MET	CA-C-N	-10.53	110.10	120.52
1	A	186	MET	C-N-CA	-10.53	110.10	120.52
2	D	32	ASP	N-CA-CB	-10.45	95.36	111.35
2	D	54	VAL	CB-CA-C	-9.34	96.36	110.55
2	D	68	ASP	CB-CA-C	-9.22	90.73	111.30
1	A	171	ALA	N-CA-C	-8.99	98.67	110.53
1	A	234	GLU	N-CA-C	8.69	122.37	109.24
1	C	204	ILE	CB-CA-C	8.56	124.08	111.33
2	B	125	TYR	CB-CA-C	8.46	123.10	109.90
2	D	51	VAL	N-CA-C	-8.36	87.59	111.00
1	C	234	GLU	N-CA-C	8.10	122.77	109.24
1	C	171	ALA	N-CA-C	-8.03	100.18	110.53
2	D	117	CYS	CB-CA-C	-7.97	94.79	109.46
1	C	151	LYS	N-CA-CB	-7.88	97.17	110.49
2	B	125	TYR	CA-CB-CG	7.80	127.94	113.90
2	D	92	ASN	N-CA-CB	7.79	123.74	110.50
1	C	152	ARG	N-CA-C	7.75	122.18	109.24
2	B	134	PRO	CB-CA-C	-7.60	104.48	111.40
1	C	247	ASP	N-CA-CB	-7.41	98.36	110.59
1	C	162	MET	N-CA-C	7.24	121.76	113.15
2	D	91	GLU	O-C-N	-7.16	113.03	122.33
1	C	234	GLU	CB-CA-C	-6.84	95.81	109.35
2	D	91	GLU	CA-C-O	-6.82	111.56	119.61
2	B	117	CYS	CB-CA-C	-6.80	96.22	109.76
2	B	88	ARG	N-CA-CB	-6.72	100.17	110.65
2	D	53	GLU	N-CA-C	-6.69	96.23	107.80
1	A	171	ALA	CA-C-N	6.68	133.72	121.70
1	A	171	ALA	C-N-CA	6.68	133.72	121.70
2	D	109	VAL	N-CA-C	-6.63	101.01	109.30
2	D	79	PRO	N-CA-C	-6.59	102.00	111.22
2	B	22	PHE	N-CA-C	-6.44	99.20	109.76
2	B	54	VAL	N-CA-C	6.42	119.54	108.95
1	A	214	TRP	CA-C-N	-6.38	112.11	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	TRP	C-N-CA	-6.38	112.11	122.82
1	A	152	ARG	N-CA-C	6.23	119.69	108.48
2	B	59	THR	CA-C-N	-6.19	111.55	122.26
2	B	59	THR	C-N-CA	-6.19	111.55	122.26
2	D	48	ALA	CA-C-N	6.16	132.80	121.70
2	D	48	ALA	C-N-CA	6.16	132.80	121.70
2	D	8	TYR	CA-C-N	6.04	133.08	121.54
2	D	8	TYR	C-N-CA	6.04	133.08	121.54
1	A	224	SER	CB-CA-C	-6.02	96.69	110.18
1	C	208	LYS	CB-CA-C	-5.98	98.61	109.38
2	D	24	ARG	CB-CG-CD	-5.94	97.65	111.30
2	D	55	TYR	N-CA-C	-5.89	99.79	109.40
1	C	186	MET	CB-CA-C	5.89	119.53	109.82
1	C	217	ILE	N-CA-C	5.83	116.40	107.77
2	D	26	LEU	CA-C-N	5.83	125.50	119.56
2	D	26	LEU	C-N-CA	5.83	125.50	119.56
1	C	203	ARG	CB-CA-C	-5.78	98.24	109.68
2	B	12	LYS	CB-CA-C	-5.77	99.61	110.51
2	B	48	ALA	CA-C-N	5.74	132.03	121.70
2	B	48	ALA	C-N-CA	5.74	132.03	121.70
2	B	125	TYR	N-CA-C	-5.73	101.56	110.10
2	D	10	LYS	CB-CA-C	5.73	121.45	110.17
2	B	53	GLU	N-CA-C	-5.68	98.69	110.80
1	C	226	LYS	CG-CD-CE	-5.67	98.26	111.30
2	D	106	ASN	N-CA-C	5.65	119.49	111.92
1	C	165	ARG	CB-CA-C	-5.64	100.37	110.70
1	C	158	ASN	N-CA-C	5.64	119.90	109.24
2	D	92	ASN	CB-CA-C	5.64	120.81	110.10
2	B	79	PRO	N-CA-C	-5.61	103.31	111.33
2	D	10	LYS	N-CA-C	5.58	122.14	109.81
1	C	187	PRO	N-CA-C	5.57	119.76	111.41
1	A	230	THR	CA-C-N	-5.54	115.07	122.72
1	A	230	THR	C-N-CA	-5.54	115.07	122.72
1	C	170	PRO	CB-CA-C	-5.53	102.72	110.63
2	D	118	LYS	N-CA-C	-5.52	102.35	110.52
1	C	162	MET	CB-CA-C	5.47	120.48	110.36
2	B	74	TYR	CA-C-N	-5.47	117.50	122.80
2	B	74	TYR	C-N-CA	-5.47	117.50	122.80
1	A	188	THR	N-CA-CB	-5.44	102.03	110.46
2	B	50	SER	N-CA-C	-5.43	101.29	109.60
2	B	39	ASP	N-CA-C	5.43	118.19	110.10
1	A	208	LYS	N-CA-CB	-5.41	101.99	110.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	GLU	N-CA-CB	5.38	118.54	109.78
1	A	169	VAL	N-CA-CB	-5.34	103.73	111.21
1	A	234	GLU	CA-CB-CG	5.33	124.77	114.10
2	B	130	ILE	CB-CA-C	-5.32	105.38	112.46
2	D	114	ASN	CA-C-N	-5.32	114.96	123.31
2	D	114	ASN	C-N-CA	-5.32	114.96	123.31
1	C	174	THR	N-CA-CB	-5.30	102.38	110.85
1	A	243	THR	CA-C-N	-5.27	114.39	122.87
1	A	243	THR	C-N-CA	-5.27	114.39	122.87
2	D	81	GLU	N-CA-C	5.26	122.00	110.80
2	D	81	GLU	CB-CG-CD	-5.25	103.68	112.60
2	B	129	ALA	CA-C-N	-5.24	114.28	122.56
2	B	129	ALA	C-N-CA	-5.24	114.28	122.56
2	D	129	ALA	CA-C-N	-5.24	114.84	122.28
2	D	129	ALA	C-N-CA	-5.24	114.84	122.28
1	A	161	LYS	CD-CE-NZ	5.24	128.65	111.90
1	C	214	TRP	CA-C-N	-5.23	114.03	122.82
1	C	214	TRP	C-N-CA	-5.23	114.03	122.82
2	D	109	VAL	CB-CA-C	-5.21	103.56	111.33
1	C	235	ASN	N-CA-CB	5.20	119.28	110.49
2	B	42	ILE	N-CA-C	5.20	117.89	112.90
2	D	26	LEU	N-CA-C	-5.16	103.44	110.36
2	D	26	LEU	CB-CA-C	5.10	117.48	109.37
2	B	113	LYS	CA-C-N	-5.10	113.79	122.56
2	B	113	LYS	C-N-CA	-5.10	113.79	122.56
2	D	22	PHE	N-CA-C	-5.06	101.45	109.59
1	A	188	THR	CB-CA-C	-5.05	101.72	110.45
1	C	165	ARG	NE-CZ-NH1	-5.02	116.48	121.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	91	GLU	CA
2	D	92	ASN	CA

There are no planarity outliers.

5.2 Too-close contacts

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	832	0	810	64	0
1	C	825	0	801	89	0
2	B	1022	0	1007	93	0
2	D	1051	0	1035	138	0
3	E	55	0	6	4	0
3	F	55	0	6	16	0
4	A	80	0	0	26	0
4	B	68	0	0	32	0
4	C	98	0	0	33	0
4	D	97	0	0	47	0
All	All	4183	0	3665	390	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 52.

All (390) 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:C:197:GLU:CG	1:C:197:GLU:CB	1.74	1.63
2:D:26:LEU:CD2	2:D:26:LEU:CG	1.82	1.57
2:D:128:LYS:CE	2:D:128:LYS:NZ	1.68	1.57
2:D:128:LYS:CE	2:D:128:LYS:CD	1.77	1.57
2:D:10:LYS:CG	2:D:11:PRO:HD3	1.07	1.51
2:B:112:LYS:CE	2:B:112:LYS:NZ	1.69	1.51
1:A:212[A]:GLN:CG	1:A:212[A]:GLN:CB	1.86	1.49
2:B:57:LYS:NZ	2:B:57:LYS:CE	1.70	1.49
1:A:196:LYS:NZ	1:A:196:LYS:CE	1.72	1.48
2:D:10:LYS:HG2	2:D:11:PRO:CD	1.00	1.47
2:D:118:LYS:NZ	2:D:118:LYS:CE	1.79	1.45
1:A:186:MET:SD	1:A:186:MET:CE	2.05	1.45
1:C:200:GLN:HG2	4:C:375:HOH:O	1.40	1.22
2:D:51:VAL:HG12	4:D:210:HOH:O	1.38	1.19
1:A:179:CYS:HB2	4:A:323:HOH:O	1.44	1.18
1:C:174:THR:HB	4:C:361:HOH:O	1.02	1.17
2:B:47:SER:CB	4:B:210:HOH:O	1.93	1.17
1:C:216:LEU:HD23	1:C:217:ILE:N	1.59	1.16
2:D:101:LYS:HE2	4:D:222:HOH:O	1.46	1.15
2:B:48:ALA:HB1	2:B:50:SER:N	1.60	1.14
1:A:151:LYS:HD2	1:A:237:TYR:OH	1.46	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:SER:HB3	4:C:356:HOH:O	1.42	1.13
1:A:174:THR:HB	4:A:306:HOH:O	0.97	1.11
1:C:174:THR:HG22	4:C:358:HOH:O	1.49	1.11
2:D:87:GLU:HG3	2:D:97:TYR:CE2	1.84	1.11
2:B:81:GLU:HG3	2:B:101:LYS:HE2	1.32	1.11
2:D:137:VAL:O	4:D:211:HOH:O	1.68	1.09
2:B:124:HIS:HA	4:B:172:HOH:O	1.51	1.08
1:C:171:ALA:HB3	4:C:372:HOH:O	0.92	1.08
1:A:172:ALA:HB1	4:A:308:HOH:O	1.53	1.06
2:D:81:GLU:HA	4:D:269:HOH:O	1.56	1.06
2:D:9:LYS:C	4:D:239:HOH:O	1.99	1.06
2:B:47:SER:HB2	4:B:210:HOH:O	1.51	1.05
2:D:10:LYS:CD	2:D:11:PRO:HD2	1.86	1.05
2:D:118:LYS:NZ	3:F:1:GU4:O26	1.91	1.04
2:D:119:ARG:HD3	4:D:254:HOH:O	1.57	1.04
2:B:43:GLN:H	2:B:43:GLN:NE2	1.58	1.02
2:D:86:LEU:HB3	2:D:88:ARG:HH22	1.23	1.00
2:B:48:ALA:HB1	2:B:50:SER:H	1.18	1.00
2:D:50:SER:HB3	2:D:51:VAL:HG22	1.00	0.99
1:C:216:LEU:C	1:C:216:LEU:CD2	2.34	0.98
2:B:43:GLN:HE21	2:B:43:GLN:N	1.60	0.98
2:D:50:SER:HB3	2:D:51:VAL:CG2	1.93	0.98
1:C:156:TRP:CD2	1:C:162:MET:HE1	2.00	0.97
2:B:124:HIS:HB2	4:B:194:HOH:O	1.63	0.96
2:D:10:LYS:CG	2:D:11:PRO:CD	1.84	0.95
1:A:164:LYS:HE2	4:A:274:HOH:O	1.65	0.95
1:C:188:THR:HG23	4:C:289:HOH:O	1.65	0.95
1:C:216:LEU:HD23	1:C:216:LEU:C	1.88	0.94
2:D:125:TYR:CD2	4:D:206:HOH:O	2.18	0.94
2:D:10:LYS:CG	2:D:11:PRO:HD2	1.94	0.94
1:C:216:LEU:CD2	1:C:217:ILE:N	2.33	0.92
1:C:212[B]:GLN:OE1	4:C:381:HOH:O	1.87	0.91
2:D:50:SER:CB	2:D:51:VAL:HG22	1.97	0.91
2:D:10:LYS:CB	2:D:11:PRO:HD3	2.03	0.89
2:D:49:GLU:HA	2:D:50:SER:OG	1.73	0.89
1:C:150:ASN:N	4:C:380:HOH:O	2.04	0.89
1:C:174:THR:CB	4:C:361:HOH:O	1.76	0.88
1:C:151:LYS:HG2	1:C:237:TYR:CZ	2.08	0.87
2:D:9:LYS:HB2	4:D:240:HOH:O	1.72	0.87
2:D:90:GLU:HB3	2:D:92:ASN:HB2	1.56	0.87
2:D:86:LEU:HB3	2:D:88:ARG:NH2	1.87	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:LYS:CD	2:D:11:PRO:CD	2.47	0.87
1:A:249:VAL:C	4:A:315:HOH:O	2.18	0.86
1:A:197:GLU:HG2	4:A:272:HOH:O	1.74	0.86
2:D:60:GLU:HB2	4:D:185:HOH:O	1.76	0.86
2:D:134:PRO:HA	4:D:264:HOH:O	1.74	0.86
2:B:72:LEU:HD23	2:B:73:LEU:O	1.76	0.86
2:B:37:ARG:HD3	4:B:171:HOH:O	1.76	0.84
2:B:128:LYS:NZ	4:B:162:HOH:O	2.02	0.83
2:D:40:GLN:NE2	4:D:221:HOH:O	2.08	0.83
2:D:10:LYS:HG2	2:D:11:PRO:CG	2.05	0.82
2:B:47:SER:HB3	4:B:210:HOH:O	1.62	0.81
2:D:10:LYS:N	4:D:239:HOH:O	2.12	0.81
1:C:216:LEU:HD23	1:C:217:ILE:H	1.46	0.81
2:B:43:GLN:H	2:B:43:GLN:HE21	0.83	0.81
2:B:43:GLN:NE2	2:B:43:GLN:N	2.22	0.80
2:B:92:ASN:HB3	2:B:94:TYR:HD2	1.44	0.80
1:A:176:LYS:HE2	3:F:2:YYJ:C1	2.12	0.79
2:B:49:GLU:HB3	4:B:197:HOH:O	1.81	0.79
2:D:11:PRO:O	2:D:137:VAL:HG23	1.83	0.79
1:C:150:ASN:HA	4:C:380:HOH:O	1.82	0.78
1:C:172:ALA:HB1	4:C:376:HOH:O	1.83	0.77
2:D:9:LYS:CA	4:D:239:HOH:O	2.29	0.77
2:D:37:ARG:NH2	4:D:215:HOH:O	2.07	0.77
2:D:14:LEU:HA	4:D:264:HOH:O	1.84	0.76
2:D:26:LEU:HD23	2:D:27:PRO:HD2	1.68	0.76
1:A:196:LYS:HB2	4:A:325:HOH:O	1.86	0.76
1:C:179:CYS:HB2	4:C:309:HOH:O	1.86	0.76
2:D:45:GLN:HG2	2:D:59:THR:HG22	1.66	0.76
2:D:10:LYS:HG2	2:D:11:PRO:HD2	1.47	0.75
4:D:259:HOH:O	3:F:2:YYJ:O1S3	2.02	0.75
2:B:37:ARG:HG2	4:B:212:HOH:O	1.86	0.75
2:B:58:SER:OG	2:B:61:THR:HG22	1.86	0.75
1:C:151:LYS:HG2	1:C:237:TYR:CE2	2.21	0.74
4:D:258:HOH:O	3:F:2:YYJ:C6	2.36	0.73
2:B:48:ALA:HB1	2:B:49:GLU:C	2.13	0.73
1:C:220:SER:CB	4:C:356:HOH:O	2.12	0.73
2:D:24:ARG:NH2	2:D:32:ASP:OD1	2.22	0.73
1:C:174:THR:CG2	4:C:358:HOH:O	2.20	0.73
1:A:199:LYS:HD3	1:A:202:HIS:CE1	2.24	0.72
2:B:93:HIS:HD2	4:B:152:HOH:O	1.70	0.72
2:D:10:LYS:HD3	2:D:11:PRO:HD2	1.69	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:TYR:CZ	4:A:298:HOH:O	2.43	0.72
2:B:48:ALA:CB	2:B:50:SER:H	2.01	0.72
1:C:216:LEU:C	1:C:216:LEU:HD22	2.14	0.72
2:D:122:ARG:HD3	3:F:1:GU4:O22	1.89	0.72
2:B:137:VAL:O	4:B:151:HOH:O	2.07	0.72
2:B:114:ASN:C	2:B:114:ASN:HD22	1.98	0.71
1:A:189:MET:HE1	1:A:214:TRP:C	2.15	0.71
1:A:164:LYS:CE	4:A:274:HOH:O	2.30	0.71
2:B:37:ARG:CG	4:B:211:HOH:O	2.38	0.71
2:D:114:ASN:C	2:D:114:ASN:HD22	1.99	0.71
2:D:134:PRO:O	4:D:265:HOH:O	2.09	0.70
2:B:19:GLY:O	2:B:35:ARG:NH2	2.23	0.70
2:D:26:LEU:CD2	2:D:26:LEU:HG	2.16	0.70
2:D:9:LYS:HA	4:D:239:HOH:O	1.88	0.70
2:B:37:ARG:CD	4:B:211:HOH:O	2.40	0.70
2:B:124:HIS:CD2	4:B:155:HOH:O	2.44	0.70
1:C:171:ALA:HB1	1:C:221:VAL:O	1.91	0.70
2:D:118:LYS:NZ	3:F:1:GU4:S4	2.63	0.69
2:B:57:LYS:HD2	4:B:168:HOH:O	1.91	0.69
1:A:207:TYR:CE2	4:A:298:HOH:O	2.44	0.69
1:C:174:THR:HG23	1:C:174:THR:O	1.92	0.69
1:C:208:LYS:CE	4:C:297:HOH:O	2.40	0.69
2:D:114:ASN:ND2	2:D:116:SER:H	1.91	0.69
2:B:50:SER:OG	2:B:52:GLY:N	2.25	0.69
2:D:82:GLU:HG3	4:D:203:HOH:O	1.92	0.69
2:D:57:LYS:HE2	2:D:62:GLY:HA2	1.75	0.69
2:B:37:ARG:HD3	4:B:212:HOH:O	1.93	0.68
1:C:150:ASN:N	1:C:150:ASN:OD1	2.25	0.68
2:B:124:HIS:HD2	4:B:155:HOH:O	1.76	0.68
2:D:79:PRO:O	2:D:80:ASN:CB	2.41	0.68
2:D:89:LEU:HD21	4:D:193:HOH:O	1.94	0.68
2:B:18:ASN:HB2	2:B:129:ALA:HA	1.76	0.67
2:D:118:LYS:NZ	3:F:1:GU4:H61	2.10	0.67
1:C:208:LYS:HE2	4:C:297:HOH:O	1.96	0.66
2:B:125:TYR:HB3	4:B:154:HOH:O	1.95	0.66
1:C:199:LYS:HE3	4:C:327:HOH:O	1.95	0.66
2:D:87:GLU:HG3	2:D:97:TYR:HE2	1.57	0.66
2:D:7:ASN:CG	2:D:8:TYR:H	2.04	0.66
1:C:175:VAL:CG2	1:C:221:VAL:HG21	2.25	0.66
2:D:18:ASN:HB2	2:D:129:ALA:HA	1.78	0.66
2:B:37:ARG:CD	4:B:212:HOH:O	2.43	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:ARG:HG2	2:D:88:ARG:HH21	1.62	0.65
2:D:8:TYR:O	2:D:12:LYS:HE2	1.97	0.65
2:D:45:GLN:HG2	2:D:59:THR:CG2	2.26	0.65
2:D:90:GLU:HG3	2:D:91:GLU:H	1.62	0.65
1:C:189:MET:HE3	1:C:191:TRP:HE1	1.62	0.65
2:D:8:TYR:O	2:D:12:LYS:CE	2.45	0.64
2:D:125:TYR:HD2	4:D:206:HOH:O	1.66	0.64
2:B:72:LEU:CD2	2:B:73:LEU:O	2.44	0.64
2:B:104:GLU:OE2	2:B:105:LYS:HD3	1.98	0.64
1:A:213:HIS:HD2	4:D:249:HOH:O	1.79	0.64
1:C:150:ASN:CA	4:C:380:HOH:O	2.35	0.63
1:C:156:TRP:CZ3	1:C:179:CYS:HB3	2.32	0.63
2:B:37:ARG:HA	4:B:211:HOH:O	1.97	0.63
2:D:48:ALA:HB1	2:D:49:GLU:HA	1.79	0.63
2:D:86:LEU:CB	2:D:88:ARG:HH22	2.06	0.63
2:D:48:ALA:HB1	2:D:50:SER:HA	1.80	0.63
2:D:14:LEU:HD23	4:D:264:HOH:O	1.98	0.63
1:A:161:LYS:HE3	1:A:178[A]:ARG:HD2	1.80	0.62
2:D:43:GLN:HB3	4:D:246:HOH:O	1.99	0.62
1:A:172:ALA:CB	4:A:308:HOH:O	2.24	0.62
2:B:48:ALA:HB1	2:B:49:GLU:CA	2.30	0.62
2:B:37:ARG:CG	4:B:212:HOH:O	2.46	0.62
2:B:104:GLU:N	2:B:104:GLU:OE1	2.33	0.62
1:C:156:TRP:CE2	1:C:162:MET:HE1	2.34	0.62
2:B:42:ILE:HD13	2:B:42:ILE:H	1.64	0.62
2:D:12:LYS:HD2	2:D:12:LYS:N	2.15	0.62
2:B:37:ARG:HD2	4:B:211:HOH:O	2.00	0.61
2:B:92:ASN:HB3	2:B:94:TYR:CD2	2.30	0.61
2:D:52:GLY:HA2	4:D:210:HOH:O	1.98	0.61
1:A:207:TYR:C	1:A:207:TYR:CD2	2.79	0.61
2:D:114:ASN:HD22	2:D:116:SER:H	1.48	0.61
1:C:220:SER:CA	4:C:356:HOH:O	2.44	0.61
2:D:122:ARG:HD2	4:D:262:HOH:O	2.00	0.60
1:C:152:ARG:HG2	4:C:371:HOH:O	2.01	0.60
2:D:18:ASN:ND2	2:D:129:ALA:HB2	2.16	0.60
2:B:61:THR:HG23	2:B:63:GLN:HG3	1.83	0.60
2:D:43:GLN:CB	4:D:246:HOH:O	2.50	0.59
1:C:201:GLU:HA	4:C:323:HOH:O	2.01	0.59
1:C:156:TRP:CE3	1:C:162:MET:HE1	2.37	0.59
1:C:161:LYS:NZ	3:E:2:YYJ:O2S3	2.35	0.59
2:B:37:ARG:HG3	4:B:211:HOH:O	2.00	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:GLN:HG2	4:B:209:HOH:O	2.02	0.58
1:A:197:GLU:HA	4:A:272:HOH:O	2.02	0.58
1:C:197:GLU:O	1:C:202:HIS:HE1	1.87	0.58
1:C:191:TRP:CE2	1:C:216:LEU:HB2	2.38	0.58
2:D:101:LYS:HD3	4:D:270:HOH:O	2.04	0.58
2:D:101:LYS:HG3	4:D:217:HOH:O	2.03	0.58
2:D:124:HIS:CE1	2:D:127:GLN:NE2	2.72	0.58
2:D:78:THR:HG23	4:D:220:HOH:O	2.02	0.57
1:A:228:ASN:CB	4:A:316:HOH:O	2.53	0.57
2:D:98:ILE:HD11	2:D:108:PHE:CE2	2.40	0.57
1:A:168:ALA:HB3	2:B:15:TYR:CE2	2.40	0.57
2:B:105:LYS:HE3	2:B:107:TRP:CZ2	2.40	0.57
2:B:81:GLU:HB2	2:B:101:LYS:HD3	1.86	0.57
2:D:107:TRP:CZ2	2:D:121:PRO:HG3	2.40	0.56
2:D:88:ARG:NH2	2:D:88:ARG:HG2	2.19	0.56
2:D:57:LYS:CE	2:D:62:GLY:HA2	2.36	0.56
1:C:158:ASN:C	1:C:158:ASN:OD1	2.46	0.56
2:D:122:ARG:NH1	4:D:207:HOH:O	2.30	0.56
2:D:49:GLU:HA	2:D:50:SER:CB	2.34	0.56
2:D:111:LEU:HD23	2:D:117:CYS:HA	1.87	0.56
1:A:154:PRO:O	4:A:250:HOH:O	2.18	0.56
1:A:189:MET:HE1	1:A:215:SER:N	2.21	0.55
2:B:14:LEU:N	2:B:14:LEU:HD12	2.21	0.55
2:D:47:SER:O	2:D:54:VAL:HA	2.06	0.55
1:C:159:THR:CG2	4:C:355:HOH:O	2.54	0.55
2:D:90:GLU:HG3	2:D:91:GLU:N	2.21	0.55
1:C:151:LYS:HE3	1:C:237:TYR:OH	2.06	0.55
2:D:46:LEU:HB3	2:D:54:VAL:HG11	1.88	0.55
2:D:137:VAL:C	4:D:209:HOH:O	2.50	0.55
1:C:171:ALA:CB	4:C:372:HOH:O	1.80	0.55
2:D:87:GLU:CG	2:D:97:TYR:CE2	2.76	0.55
3:E:1:GU4:S4	3:E:1:GU4:H61	2.47	0.55
1:A:233:VAL:O	1:A:239:SER:HA	2.07	0.54
1:A:188:THR:HG22	1:A:189:MET:N	2.21	0.54
1:C:171:ALA:CB	1:C:221:VAL:O	2.55	0.54
1:C:228:ASN:OD1	1:C:245[B]:HIS:HD2	1.90	0.54
1:A:228:ASN:HB3	4:A:316:HOH:O	2.08	0.54
2:B:36:ASP:OD1	2:B:38:SER:HB3	2.07	0.54
1:C:156:TRP:HZ3	1:C:179:CYS:HB3	1.73	0.54
2:D:81:GLU:HB3	4:D:203:HOH:O	2.06	0.54
3:E:1:GU4:H5	3:E:2:YYJ:O5	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:HD3	1:A:178[A]:ARG:HH21	1.73	0.53
1:A:189:MET:HE3	1:A:191:TRP:HE1	1.74	0.53
2:D:134:PRO:HD2	4:D:265:HOH:O	2.08	0.53
2:D:79:PRO:O	2:D:80:ASN:HB2	2.08	0.53
1:C:175:VAL:HG23	1:C:221:VAL:HG21	1.91	0.53
1:C:151:LYS:CE	1:C:237:TYR:OH	2.57	0.52
1:A:161:LYS:HE3	1:A:178[B]:ARG:HD3	1.90	0.52
1:C:189:MET:CE	1:C:191:TRP:HE1	2.22	0.52
1:A:178[B]:ARG:NH1	1:A:180:PRO:HG3	2.24	0.52
1:A:236:GLU:OE1	1:A:236:GLU:N	2.39	0.52
1:C:174:THR:OG1	4:C:361:HOH:O	2.05	0.52
2:B:88:ARG:HH21	2:B:88:ARG:HG3	1.75	0.52
2:B:90:GLU:C	2:B:92:ASN:H	2.17	0.52
1:A:208:LYS:HG3	4:A:307:HOH:O	2.09	0.52
2:B:137:VAL:O	2:B:137:VAL:HG12	2.09	0.52
2:D:114:ASN:C	2:D:114:ASN:ND2	2.68	0.52
1:C:159:THR:HG22	4:C:355:HOH:O	2.10	0.51
2:D:78:THR:CG2	4:D:220:HOH:O	2.57	0.51
2:D:128:LYS:CE	2:D:128:LYS:CG	2.81	0.51
1:C:151:LYS:CG	1:C:237:TYR:OH	2.58	0.51
2:D:89:LEU:HD11	2:D:93:HIS:HB3	1.92	0.51
2:D:92:ASN:HB3	2:D:94:TYR:H	1.75	0.51
1:A:180:PRO:HB3	1:C:160:GLU:OE2	2.10	0.51
2:B:49:GLU:HG2	2:B:50:SER:O	2.10	0.51
2:D:13:LEU:HD22	2:D:42:ILE:HG13	1.92	0.51
2:B:67:MET:HG3	2:B:73:LEU:HD23	1.93	0.51
2:B:112:LYS:NZ	2:B:112:LYS:CD	2.61	0.51
2:D:28:ASP:OD1	2:D:30:THR:HG23	2.11	0.51
2:D:90:GLU:HB3	2:D:92:ASN:CB	2.37	0.51
2:D:137:VAL:O	2:D:137:VAL:HG12	2.11	0.51
1:C:191:TRP:CZ3	1:C:231:CYS:HB3	2.46	0.50
1:C:197:GLU:O	1:C:202:HIS:CE1	2.65	0.50
1:A:246:LEU:HD22	1:A:247:ASP:N	2.27	0.50
2:D:51:VAL:CG1	4:D:210:HOH:O	2.20	0.50
1:A:158:ASN:N	4:A:309:HOH:O	2.31	0.50
2:B:37:ARG:CD	4:B:171:HOH:O	2.48	0.50
2:D:137:VAL:O	4:D:209:HOH:O	2.20	0.50
3:F:1:GU4:S4	3:F:1:GU4:O29	2.69	0.50
1:C:180:PRO:HA	1:C:214:TRP:CD1	2.48	0.49
1:A:158:ASN:C	4:A:309:HOH:O	2.56	0.49
1:C:249:VAL:C	4:C:357:HOH:O	2.54	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:HD3	3:F:1:GU4:O10	2.13	0.49
2:D:48:ALA:CB	2:D:49:GLU:HA	2.42	0.49
1:C:176:LYS:NZ	4:C:365:HOH:O	2.44	0.49
2:D:88:ARG:HH21	2:D:88:ARG:CG	2.24	0.49
3:E:1:GU4:H62	3:E:2:YYJ:O3S1	2.13	0.49
1:A:151:LYS:HB3	1:A:237:TYR:CE2	2.47	0.49
2:D:11:PRO:O	2:D:137:VAL:CG2	2.57	0.49
2:D:49:GLU:CA	2:D:50:SER:OG	2.55	0.49
2:D:98:ILE:HG12	2:D:108:PHE:CD2	2.48	0.49
2:B:136:PRO:HD2	4:B:142:HOH:O	2.13	0.48
2:D:49:GLU:OE2	2:D:49:GLU:O	2.31	0.48
2:D:122:ARG:HD3	3:F:1:GU4:S6	2.53	0.48
1:C:151:LYS:CG	1:C:237:TYR:CZ	2.91	0.48
2:B:92:ASN:HB2	2:B:94:TYR:H	1.78	0.48
1:C:156:TRP:CD2	1:C:162:MET:CE	2.87	0.48
1:C:225:ASP:O	1:C:226:LYS:C	2.56	0.48
2:B:13:LEU:HD22	2:B:42:ILE:HG12	1.95	0.48
1:C:226:LYS:HG2	4:C:344:HOH:O	2.13	0.48
2:D:47:SER:H	2:D:54:VAL:HG12	1.78	0.48
2:D:117:CYS:CB	4:D:257:HOH:O	2.61	0.48
2:B:47:SER:O	2:B:54:VAL:HA	2.13	0.48
1:A:159:THR:O	1:A:160:GLU:C	2.57	0.48
1:C:203:ARG:NH1	1:C:206:GLY:O	2.43	0.48
2:D:101:LYS:HB2	4:D:251:HOH:O	2.13	0.48
2:D:124:HIS:NE2	2:D:127:GLN:NE2	2.60	0.48
2:D:40:GLN:O	2:D:60:GLU:HG3	2.13	0.47
2:D:49:GLU:HG2	2:D:50:SER:HB2	1.95	0.47
2:D:114:ASN:ND2	2:D:116:SER:OG	2.41	0.47
4:D:250:HOH:O	3:F:2:YYJ:C6	2.62	0.47
1:C:174:THR:CG2	1:C:174:THR:O	2.59	0.47
1:C:188:THR:HB	4:C:373:HOH:O	2.14	0.47
2:D:112:LYS:HG2	3:F:1:GU4:O24	2.15	0.47
1:C:158:ASN:OD1	1:C:158:ASN:O	2.32	0.47
2:D:67:MET:HB3	4:D:224:HOH:O	2.13	0.47
1:C:236:GLU:HG2	4:C:300:HOH:O	2.15	0.47
2:B:79:PRO:O	2:B:80:ASN:CB	2.61	0.47
2:D:48:ALA:C	4:D:241:HOH:O	2.58	0.47
1:A:188:THR:CG2	1:A:189:MET:N	2.78	0.46
2:B:93:HIS:CD2	4:B:152:HOH:O	2.56	0.46
1:A:191:TRP:CH2	1:A:231:CYS:HB3	2.50	0.46
1:C:152:ARG:CG	4:C:371:HOH:O	2.59	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:ASP:OD2	2:D:33:GLY:N	2.48	0.46
2:B:48:ALA:HB1	2:B:49:GLU:HA	1.97	0.46
1:C:218:MET:HE1	1:C:229:TYR:CE2	2.50	0.46
2:D:103:ALA:C	2:D:105:LYS:H	2.24	0.46
2:B:11:PRO:O	2:B:137:VAL:HG23	2.16	0.46
1:A:170:PRO:HD2	1:A:173:ASN:HD22	1.80	0.46
2:B:64:TYR:O	2:B:75:GLY:HA2	2.15	0.46
1:C:151:LYS:HG2	1:C:237:TYR:OH	2.16	0.46
2:D:8:TYR:O	2:D:12:LYS:HE3	2.16	0.46
1:C:203:ARG:NH2	1:C:219:GLU:O	2.44	0.46
2:B:91:GLU:CG	4:B:193:HOH:O	2.64	0.45
1:A:189:MET:CE	1:A:214:TRP:C	2.88	0.45
2:B:114:ASN:C	2:B:114:ASN:ND2	2.64	0.45
2:B:15:TYR:O	2:B:132:PHE:HA	2.17	0.45
2:B:48:ALA:CB	2:B:50:SER:N	2.54	0.45
2:B:91:GLU:HG3	4:B:193:HOH:O	2.16	0.45
2:B:88:ARG:HB3	2:B:96:THR:OG1	2.16	0.45
1:C:172:ALA:HA	4:C:351:HOH:O	2.15	0.45
1:C:246:LEU:HA	1:C:246:LEU:HD12	1.64	0.45
2:D:117:CYS:HB2	4:D:257:HOH:O	2.16	0.45
1:A:157:THR:HB	1:C:159:THR:HG22	1.99	0.45
1:C:213:HIS:O	1:C:214:TRP:HB2	2.17	0.45
1:A:245[B]:HIS:CD2	4:A:265:HOH:O	2.69	0.45
2:B:90:GLU:O	2:B:92:ASN:N	2.44	0.45
2:B:102:HIS:C	2:B:104:GLU:OE1	2.60	0.45
2:D:12:LYS:N	2:D:12:LYS:CD	2.80	0.45
1:C:191:TRP:CH2	1:C:231:CYS:HB3	2.52	0.45
1:A:225:ASP:O	1:A:226:LYS:C	2.61	0.44
2:B:40:GLN:HG3	4:B:182:HOH:O	2.17	0.44
1:C:175:VAL:HG23	1:C:221:VAL:CG2	2.47	0.44
2:D:45:GLN:CG	2:D:59:THR:HG22	2.43	0.44
1:A:234:GLU:HB3	1:A:239:SER:HB3	1.99	0.44
2:D:100:LYS:HD3	2:D:100:LYS:C	2.43	0.44
2:D:48:ALA:HA	2:D:53:GLU:O	2.17	0.44
1:C:178:ARG:NH2	1:C:180:PRO:HG3	2.31	0.44
2:B:105:LYS:HB2	2:B:105:LYS:HE2	1.57	0.44
2:D:118:LYS:CE	3:F:1:GU4:H61	2.48	0.44
2:B:98:ILE:O	2:B:99:SER:C	2.60	0.43
1:C:158:ASN:O	1:C:158:ASN:CG	2.58	0.43
1:A:199:LYS:HB3	4:A:318:HOH:O	2.17	0.43
2:D:43:GLN:OE1	2:D:43:GLN:N	2.45	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:GLY:N	4:D:190:HOH:O	2.45	0.43
3:F:1:GU4:O29	3:F:1:GU4:O25	2.36	0.43
2:D:118:LYS:HZ2	3:F:1:GU4:H61	1.83	0.43
1:A:164:LYS:HD3	1:A:167:HIS:NE2	2.34	0.42
1:A:247:ASP:C	1:A:247:ASP:OD1	2.63	0.42
2:B:48:ALA:CB	2:B:49:GLU:CA	2.96	0.42
4:D:247:HOH:O	3:F:2:YYJ:O4	2.21	0.42
2:B:26:LEU:HG	4:B:207:HOH:O	2.19	0.42
2:D:68:ASP:OD1	2:D:72:LEU:HB3	2.19	0.42
2:B:92:ASN:CB	2:B:94:TYR:HD2	2.23	0.42
1:A:223:PRO:HD2	4:A:313:HOH:O	2.20	0.42
1:A:172:ALA:O	1:A:220:SER:HA	2.19	0.42
1:A:194:ASN:HA	4:A:275:HOH:O	2.19	0.42
1:A:208:LYS:CE	4:A:307:HOH:O	2.67	0.42
2:B:98:ILE:HD11	2:B:108:PHE:CE2	2.55	0.41
2:B:106:ASN:HD22	2:B:106:ASN:HA	1.69	0.41
1:A:152:ARG:HG3	4:A:260:HOH:O	2.19	0.41
2:B:34:THR:HA	4:B:195:HOH:O	2.20	0.41
1:C:212[B]:GLN:CD	4:C:381:HOH:O	2.50	0.41
2:D:14:LEU:CD2	4:D:264:HOH:O	2.62	0.41
1:A:151:LYS:HD2	1:A:237:TYR:HH	1.71	0.41
2:B:31:VAL:O	2:B:117:CYS:SG	2.79	0.41
2:B:92:ASN:CB	2:B:94:TYR:H	2.33	0.41
1:C:226:LYS:HB2	1:C:226:LYS:HE2	1.53	0.41
2:D:72:LEU:HD12	2:D:73:LEU:N	2.35	0.41
2:D:96:THR:HG22	2:D:130:ILE:O	2.21	0.41
1:A:158:ASN:C	1:A:158:ASN:OD1	2.63	0.41
1:A:208:LYS:CD	4:A:307:HOH:O	2.68	0.41
1:A:208:LYS:HE3	4:A:307:HOH:O	2.21	0.41
2:B:90:GLU:C	2:B:92:ASN:N	2.78	0.41
2:D:14:LEU:O	2:D:22:PHE:HA	2.20	0.41
2:B:86:LEU:HD21	2:B:100:LYS:HD3	2.02	0.41
2:B:10:LYS:HE3	2:B:10:LYS:HB3	1.78	0.40
2:B:128:LYS:HA	2:B:128:LYS:HD2	1.91	0.40
1:C:180:PRO:HA	1:C:214:TRP:CG	2.57	0.40
1:C:199:LYS:HB3	1:C:199:LYS:HE2	1.86	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	101/100 (101%)	98 (97%)	3 (3%)	0	100	100
1	C	100/100 (100%)	93 (93%)	7 (7%)	0	100	100
2	B	126/131 (96%)	113 (90%)	11 (9%)	2 (2%)	7	16
2	D	129/131 (98%)	114 (88%)	9 (7%)	6 (5%)	2	2
All	All	456/462 (99%)	418 (92%)	30 (7%)	8 (2%)	6	14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	10	LYS
2	D	92	ASN
2	B	52	GLY
2	D	50	SER
2	D	80	ASN
2	D	9	LYS
2	B	50	SER
2	D	12	LYS

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	91/88 (103%)	82 (90%)	9 (10%)	7	16
1	C	90/88 (102%)	85 (94%)	5 (6%)	19	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	112/115 (97%)	98 (88%)	14 (12%)	4	9
2	D	115/115 (100%)	96 (84%)	19 (16%)	2	4
All	All	408/406 (100%)	361 (88%)	47 (12%)	5	11

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	THR
1	A	186	MET
1	A	199	LYS
1	A	201	GLU
1	A	212[A]	GLN
1	A	212[B]	GLN
1	A	221	VAL
1	A	226	LYS
1	A	246	LEU
2	B	38	SER
2	B	39	ASP
2	B	42	ILE
2	B	43	GLN
2	B	50	SER
2	B	58	SER
2	B	60	GLU
2	B	67	MET
2	B	80	ASN
2	B	81	GLU
2	B	84	LEU
2	B	101	LYS
2	B	104	GLU
2	B	114	ASN
1	C	159	THR
1	C	175	VAL
1	C	216	LEU
1	C	221	VAL
1	C	240	ILE
2	D	9	LYS
2	D	10	LYS
2	D	12	LYS
2	D	26	LEU
2	D	32	ASP
2	D	34	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	46	LEU
2	D	49	GLU
2	D	51	VAL
2	D	54	VAL
2	D	63	GLN
2	D	78	THR
2	D	80	ASN
2	D	88	ARG
2	D	100	LYS
2	D	105	LYS
2	D	114	ASN
2	D	117	CYS
2	D	137	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	242	HIS
2	B	43	GLN
2	B	102	HIS
2	B	106	ASN
2	B	114	ASN
1	C	150	ASN
1	C	167	HIS
1	C	173	ASN
1	C	202	HIS
1	C	242	HIS
2	D	40	GLN
2	D	45	GLN
2	D	80	ASN
2	D	92	ASN
2	D	114	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 ⓘ

4 monosaccharides 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	GU4	E	1	3	27,27,28	1.56	6 (22%)	32,43,45	2.19	10 (31%)
3	YYJ	E	2	3	27,28,28	2.79	8 (29%)	33,46,46	2.89	12 (36%)
3	GU4	F	1	3	27,27,28	2.37	9 (33%)	32,43,45	3.28	11 (34%)
3	YYJ	F	2	3	27,28,28	2.23	7 (25%)	33,46,46	2.20	6 (18%)

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	GU4	E	1	3	-	11/21/38/41	0/1/1/1
3	YYJ	E	2	3	-	10/23/42/42	0/1/1/1
3	GU4	F	1	3	-	16/21/38/41	0/1/1/1
3	YYJ	F	2	3	-	13/23/42/42	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	YYJ	O3-S3	6.43	1.76	1.57
3	E	2	YYJ	O6-S6	6.20	1.73	1.56
3	E	2	YYJ	O1-S1	6.18	1.73	1.56
3	F	1	GU4	O2-S2	5.75	1.74	1.57
3	F	2	YYJ	O6-S6	5.42	1.71	1.56
3	E	2	YYJ	O4-S4	5.28	1.73	1.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	GU4	O3-S3	5.19	1.72	1.57
3	F	2	YYJ	O2-C2	4.98	1.49	1.40
3	F	2	YYJ	O1-S1	4.72	1.69	1.56
3	F	2	YYJ	O4-S4	4.07	1.69	1.57
3	F	1	GU4	O2-C2	4.01	1.53	1.47
3	E	2	YYJ	O3-C3	3.75	1.54	1.47
3	F	1	GU4	O5-C1	-3.58	1.37	1.43
3	F	1	GU4	O5-C5	-3.55	1.36	1.43
3	E	1	GU4	O2-S2	3.55	1.68	1.57
3	F	2	YYJ	O3-S3	3.48	1.67	1.57
3	F	1	GU4	O4-S4	3.32	1.67	1.57
3	F	1	GU4	O28-S3	2.91	1.58	1.45
3	F	1	GU4	C3-C2	2.72	1.60	1.52
3	E	1	GU4	O3-S3	2.53	1.64	1.57
3	E	2	YYJ	O5-C2	2.47	1.47	1.43
3	F	2	YYJ	O2S6-S6	2.39	1.55	1.45
3	E	1	GU4	O3-C3	-2.38	1.41	1.46
3	E	1	GU4	C1-C2	2.34	1.55	1.51
3	E	2	YYJ	O2-C2	2.31	1.44	1.40
3	F	1	GU4	O24-S4	-2.18	1.37	1.50
3	E	1	GU4	O4-S4	2.15	1.63	1.57
3	F	2	YYJ	O2S3-S3	2.10	1.54	1.45
3	E	2	YYJ	C6-C5	2.01	1.57	1.51
3	E	1	GU4	O27-S3	2.01	1.54	1.45

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	GU4	O2-C2-C3	14.70	122.93	106.65
3	E	2	YYJ	C3-O3-S3	12.38	133.00	117.69
3	F	2	YYJ	C3-O3-S3	8.55	128.26	117.69
3	E	1	GU4	O2-C2-C3	7.81	115.29	106.65
3	E	2	YYJ	C4-O4-S4	4.65	130.19	119.04
3	F	2	YYJ	C4-O4-S4	4.55	129.96	119.04
3	F	1	GU4	O5-C5-C6	-4.55	97.75	107.59
3	F	2	YYJ	O3-C3-C4	4.34	121.25	109.27
3	E	2	YYJ	O4-C4-C3	4.24	118.14	108.91
3	F	1	GU4	O3-C3-C4	-4.11	99.58	108.56
3	F	2	YYJ	O4-C4-C3	3.58	116.70	108.91
3	E	2	YYJ	O1S6-S6-O6	3.36	114.09	106.37
3	F	1	GU4	O5-C1-C2	-3.33	102.77	109.51
3	F	1	GU4	O6-S6-O22	3.24	116.81	106.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	GU4	C4-O4-S4	3.18	126.67	119.04
3	F	1	GU4	O6-S6-O23	-3.08	97.50	106.92
3	E	2	YYJ	O3-C3-C4	3.07	117.76	109.27
3	E	1	GU4	C1-C2-C3	-3.03	104.86	109.40
3	E	1	GU4	O24-S4-O26	2.85	118.54	108.56
3	E	2	YYJ	O5-C5-C6	2.85	116.21	109.50
3	E	1	GU4	C3-O3-S3	2.79	125.72	119.04
3	E	2	YYJ	O5-C5-C4	2.74	107.98	103.54
3	F	1	GU4	C3-O3-S3	2.70	125.51	119.04
3	E	1	GU4	O29-S3-O3	-2.66	100.27	106.37
3	E	2	YYJ	O1S1-S1-O1	2.59	112.32	106.37
3	E	1	GU4	O6-S6-O22	2.52	114.63	106.92
3	F	1	GU4	C3-C4-C5	2.45	115.59	110.58
3	F	2	YYJ	O1S3-S3-O3	2.42	111.94	106.37
3	E	1	GU4	O5-C5-C4	2.30	114.19	110.06
3	E	2	YYJ	O2-C2-C3	-2.24	102.75	109.74
3	E	1	GU4	C1-O5-C5	-2.19	109.25	112.19
3	E	1	GU4	O5-C5-C6	-2.15	102.94	107.59
3	E	2	YYJ	O2-C2-O5	-2.13	105.24	109.33
3	E	2	YYJ	O1-S1-O3S1	2.12	113.39	106.92
3	E	2	YYJ	O6-S6-O3S6	2.10	113.33	106.92
3	F	1	GU4	O6-C6-C5	-2.10	103.83	107.57
3	E	1	GU4	O23-S6-O22	-2.09	104.19	112.24
3	F	1	GU4	O24-S4-O26	2.07	115.79	108.56
3	F	2	YYJ	O1S1-S1-O1	2.01	110.99	106.37

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	GU4	C5-C4-O4-S4
3	E	1	GU4	C1-C2-O2-S2
3	E	1	GU4	C2-O2-S2-O12
3	E	2	YYJ	O1-C1-C2-C3
3	E	2	YYJ	O1-C1-C2-O2
3	E	2	YYJ	O1-C1-C2-O5
3	E	2	YYJ	C2-C1-O1-S1
3	E	2	YYJ	C4-C3-O3-S3
3	E	2	YYJ	C3-C4-O4-S4
3	E	2	YYJ	C4-C5-C6-O6
3	E	2	YYJ	O5-C5-C6-O6
3	E	2	YYJ	C5-C6-O6-S6

Continued on next page...

Continued from previous page...

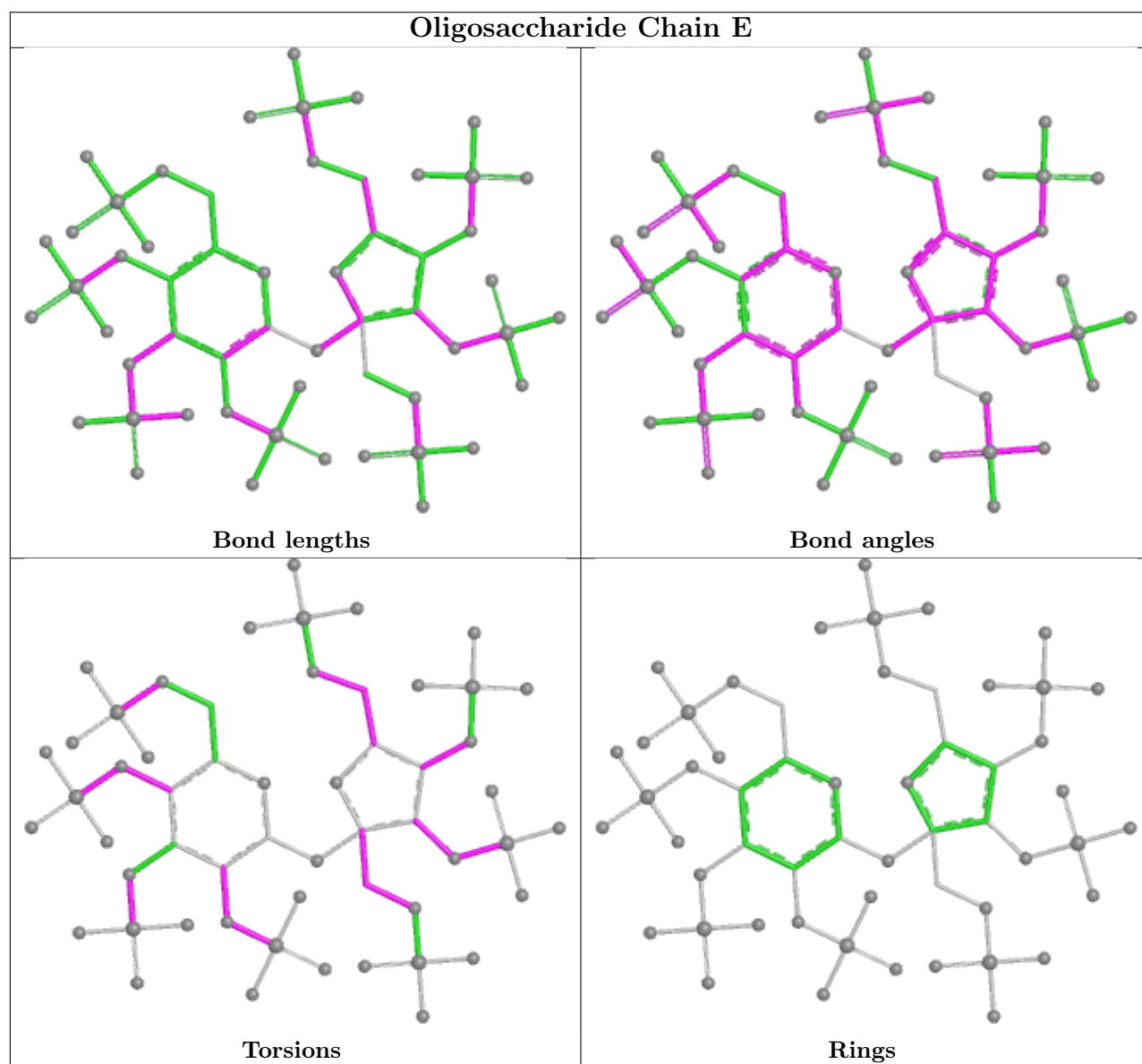
Mol	Chain	Res	Type	Atoms
3	F	1	GU4	O5-C5-C6-O6
3	F	1	GU4	C5-C4-O4-S4
3	F	1	GU4	C4-O4-S4-O26
3	F	1	GU4	C4-C3-O3-S3
3	F	1	GU4	C1-C2-O2-S2
3	F	1	GU4	C3-C2-O2-S2
3	F	2	YYJ	O1-C1-C2-C3
3	F	2	YYJ	C2-C1-O1-S1
3	F	2	YYJ	C4-C3-O3-S3
3	F	2	YYJ	C3-C4-O4-S4
3	F	2	YYJ	O5-C5-C6-O6
3	F	2	YYJ	C5-C6-O6-S6
3	F	2	YYJ	C1-O1-S1-O1S1
3	E	1	GU4	C2-O2-S2-O11
3	F	1	GU4	C4-O4-S4-O25
3	F	1	GU4	C2-O2-S2-O11
3	F	1	GU4	C2-O2-S2-O12
3	F	2	YYJ	C1-O1-S1-O2S1
3	F	2	YYJ	C1-O1-S1-O3S1
3	E	1	GU4	C2-O2-S2-O10
3	F	1	GU4	C4-O4-S4-O24
3	F	1	GU4	C2-O2-S2-O10
3	F	2	YYJ	C4-O4-S4-O1S4
3	E	1	GU4	C6-O6-S6-O21
3	F	1	GU4	C6-O6-S6-O21
3	E	1	GU4	C6-O6-S6-O23
3	E	1	GU4	C6-O6-S6-O22
3	F	1	GU4	C6-O6-S6-O22
3	F	1	GU4	C2-C3-O3-S3
3	F	1	GU4	C4-C5-C6-O6
3	E	1	GU4	C4-O4-S4-O25
3	E	1	GU4	C4-O4-S4-O26
3	E	1	GU4	C3-O3-S3-O29
3	E	2	YYJ	C3-O3-S3-O1S3
3	F	1	GU4	C6-O6-S6-O23
3	F	2	YYJ	C4-O4-S4-O2S4
3	F	2	YYJ	C3-O3-S3-O1S3
3	F	2	YYJ	C4-O4-S4-O3S4

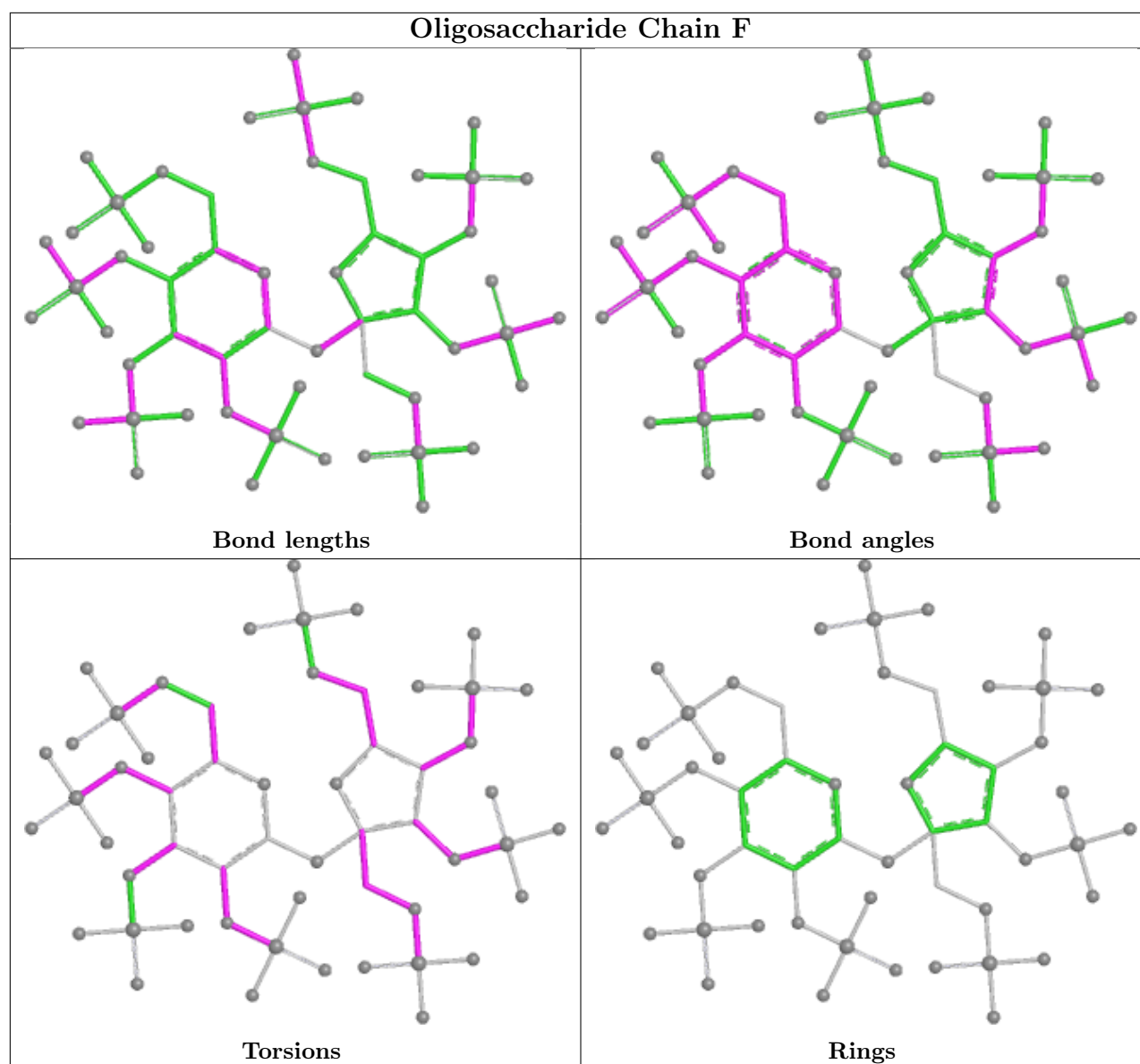
There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	GU4	11	0
3	E	1	GU4	3	0
3	F	2	YYJ	5	0
3	E	2	YYJ	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	100/100 (100%)	0.19	4 (4%)	42	37	4, 9, 15, 29	3 (3%)
1	C	100/100 (100%)	0.33	4 (4%)	42	37	3, 9, 15, 23	2 (2%)
2	B	128/131 (97%)	0.21	3 (2%)	61	55	2, 10, 17, 21	1 (0%)
2	D	131/131 (100%)	0.25	6 (4%)	37	32	5, 11, 17, 22	1 (0%)
All	All	459/462 (99%)	0.24	17 (3%)	45	39	2, 10, 17, 29	7 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	9	LYS	4.1
1	A	212[A]	GLN	3.6
1	C	201	GLU	3.5
2	B	49	GLU	3.5
2	D	7	ASN	3.5
2	D	51	VAL	3.2
2	D	104	GLU	3.1
1	A	201	GLU	2.9
1	A	150	ASN	2.8
2	B	125	TYR	2.7
2	D	91	GLU	2.7
2	D	8	TYR	2.6
1	C	199	LYS	2.3
1	C	197	GLU	2.2
2	B	88	ARG	2.1
1	A	186	MET	2.1
1	C	150	ASN	2.0

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

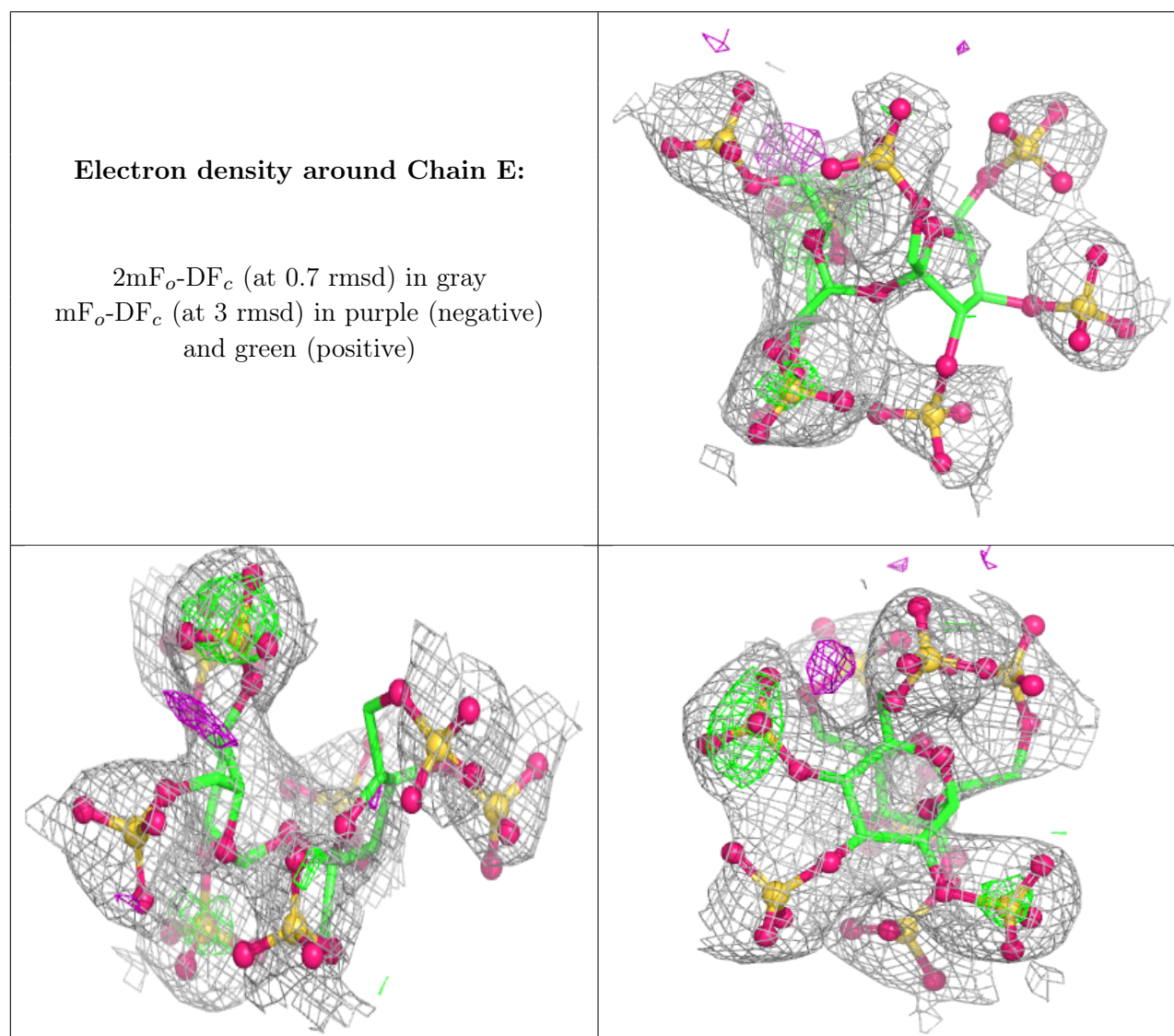
There are no non-standard protein/DNA/RNA residues in this entry.

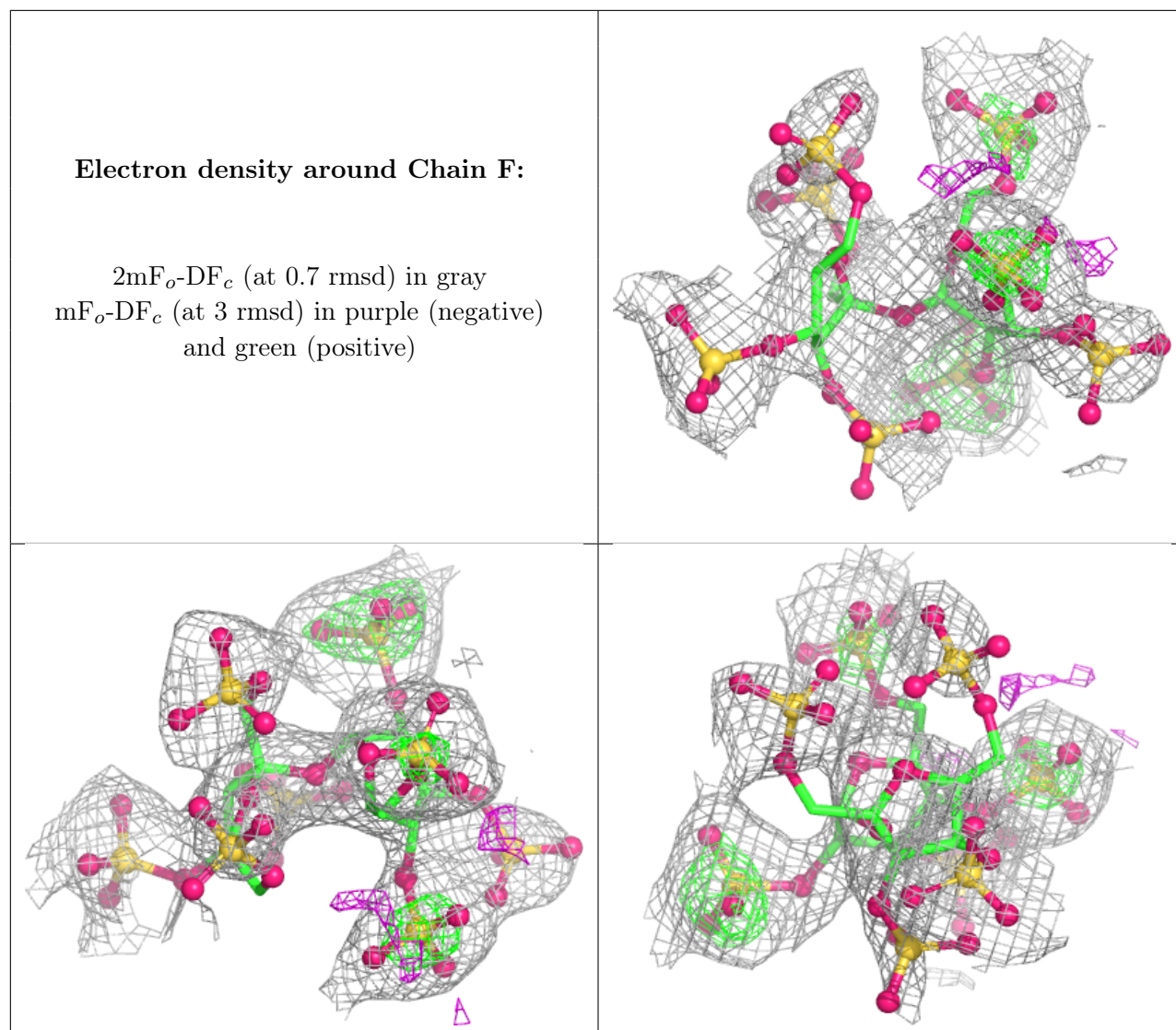
6.3 Carbohydrates [i](#)

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
3	YYJ	F	2	28/28	0.74	0.17	101,113,114,115	0
3	YYJ	E	2	28/28	0.79	0.17	102,113,115,115	0
3	GU4	F	1	27/28	0.86	0.21	71,83,88,92	0
3	GU4	E	1	27/28	0.90	0.18	73,85,90,94	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.