



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:32 PM UTC

PDB ID : 5XEX / pdb_00005xex
Title : Crystal structure of S.aureus PNPase catalytic domain
Authors : Wang, X.; Zhang, X.; Zang, J.
Deposited on : 2017-04-06
Resolution : 2.20 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

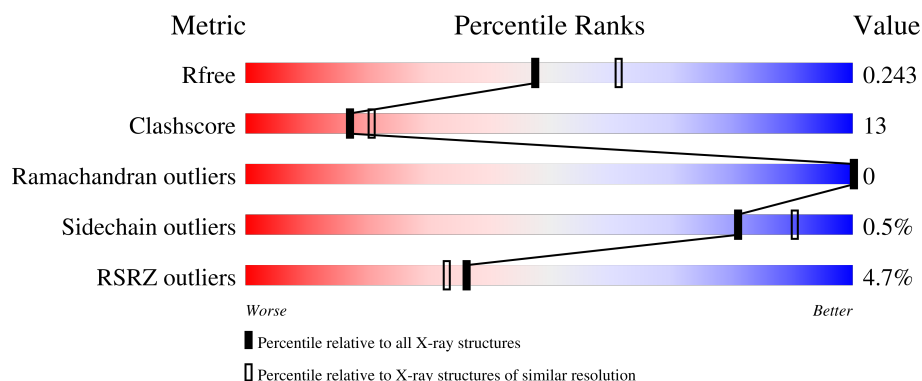
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	559	3% 68% 23% 9%
1	B	559	3% 69% 22% 9%
1	C	559	4% 69% 22% 9%
1	D	559	4% 69% 23% 8%
1	E	559	7% 69% 23% 9%

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Mol	Chain	Length	Quality of chain
1	F	559	

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
4	PPV	A	603[B]	-	-	X	-
4	PPV	B	603[A]	-	-	X	-
4	PPV	E	603[A]	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24313 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 Polyribonucleotide nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			3976	2497	684	777	18			
1	B	510	Total	C	N	O	S	0	0	0
			3970	2493	682	777	18			
1	C	511	Total	C	N	O	S	0	0	0
			3974	2495	683	778	18			
1	D	515	Total	C	N	O	S	0	0	0
			4007	2515	688	786	18			
1	E	511	Total	C	N	O	S	0	0	0
			3971	2493	683	777	18			
1	F	513	Total	C	N	O	S	0	0	0
			3987	2503	686	780	18			

There are 36 discrepancies between the modelled and reference sequences:

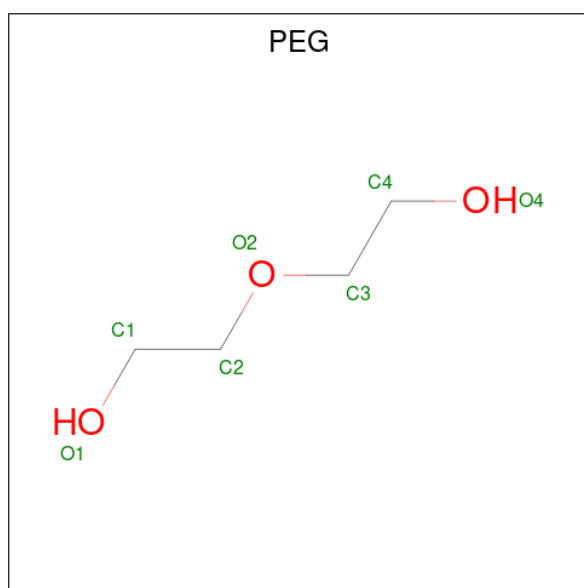
Chain	Residue	Modelled	Actual	Comment	Reference
A	554	HIS	-	expression tag	UNP Q2FZ20
A	555	HIS	-	expression tag	UNP Q2FZ20
A	556	HIS	-	expression tag	UNP Q2FZ20
A	557	HIS	-	expression tag	UNP Q2FZ20
A	558	HIS	-	expression tag	UNP Q2FZ20
A	559	HIS	-	expression tag	UNP Q2FZ20
B	554	HIS	-	expression tag	UNP Q2FZ20
B	555	HIS	-	expression tag	UNP Q2FZ20
B	556	HIS	-	expression tag	UNP Q2FZ20
B	557	HIS	-	expression tag	UNP Q2FZ20
B	558	HIS	-	expression tag	UNP Q2FZ20
B	559	HIS	-	expression tag	UNP Q2FZ20
C	554	HIS	-	expression tag	UNP Q2FZ20
C	555	HIS	-	expression tag	UNP Q2FZ20
C	556	HIS	-	expression tag	UNP Q2FZ20
C	557	HIS	-	expression tag	UNP Q2FZ20
C	558	HIS	-	expression tag	UNP Q2FZ20

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Chain	Residue	Modelled	Actual	Comment	Reference
C	559	HIS	-	expression tag	UNP Q2FZ20
D	554	HIS	-	expression tag	UNP Q2FZ20
D	555	HIS	-	expression tag	UNP Q2FZ20
D	556	HIS	-	expression tag	UNP Q2FZ20
D	557	HIS	-	expression tag	UNP Q2FZ20
D	558	HIS	-	expression tag	UNP Q2FZ20
D	559	HIS	-	expression tag	UNP Q2FZ20
E	554	HIS	-	expression tag	UNP Q2FZ20
E	555	HIS	-	expression tag	UNP Q2FZ20
E	556	HIS	-	expression tag	UNP Q2FZ20
E	557	HIS	-	expression tag	UNP Q2FZ20
E	558	HIS	-	expression tag	UNP Q2FZ20
E	559	HIS	-	expression tag	UNP Q2FZ20
F	554	HIS	-	expression tag	UNP Q2FZ20
F	555	HIS	-	expression tag	UNP Q2FZ20
F	556	HIS	-	expression tag	UNP Q2FZ20
F	557	HIS	-	expression tag	UNP Q2FZ20
F	558	HIS	-	expression tag	UNP Q2FZ20
F	559	HIS	-	expression tag	UNP Q2FZ20

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

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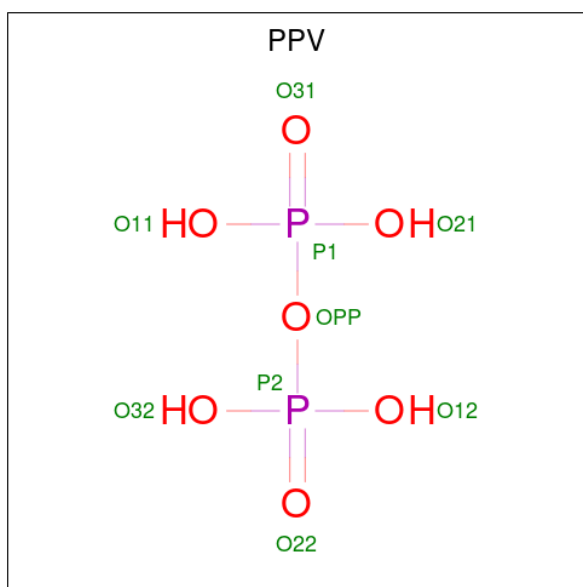
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PYROPHOSPHATE (CCD ID: PPV) (formula: $H_4O_7P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	1
			18	14	4		
4	B	1	Total	O	P	0	1
			18	14	4		
4	C	1	Total	O	P	0	1
			18	14	4		
4	D	1	Total	O	P	0	1
			18	14	4		
4	E	1	Total	O	P	0	1
			18	14	4		
4	F	1	Total	O	P	0	1
			18	14	4		

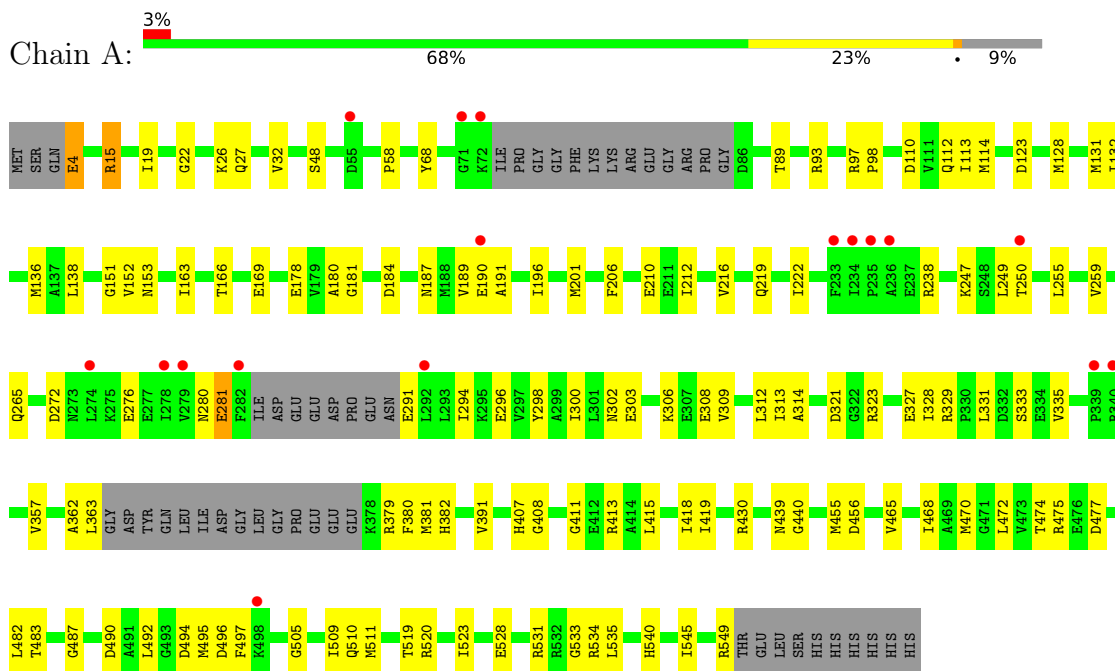
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	29	Total	O	0	0
			29	29		
5	B	17	Total	O	0	0
			17	17		
5	C	44	Total	O	0	0
			44	44		
5	D	42	Total	O	0	0
			42	42		
5	E	51	Total	O	0	0
			51	51		
5	F	59	Total	O	0	0
			59	59		

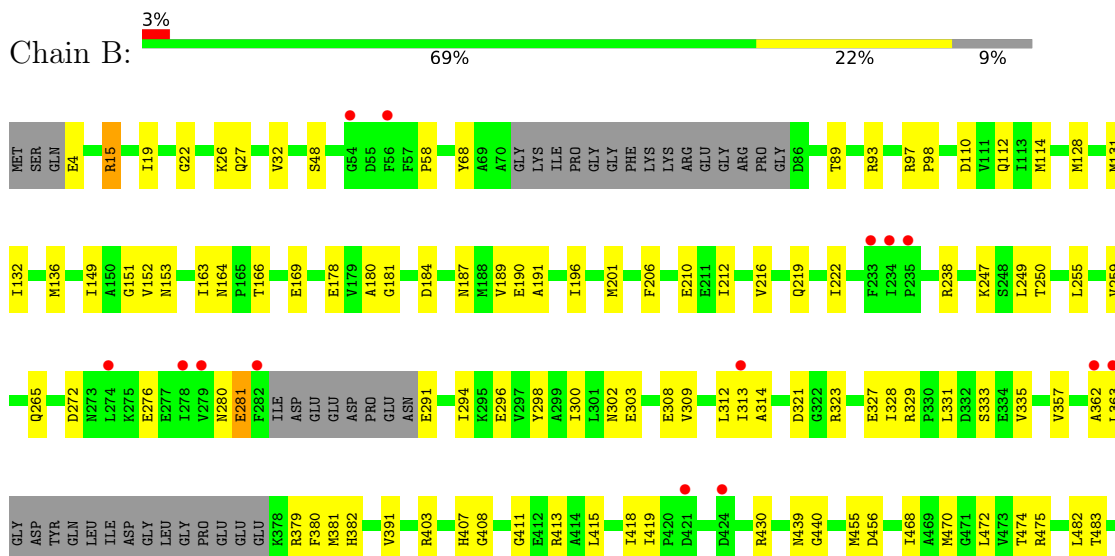
3 Residue-property plots [i](#)

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: Polyribonucleotide nucleotidyltransferase

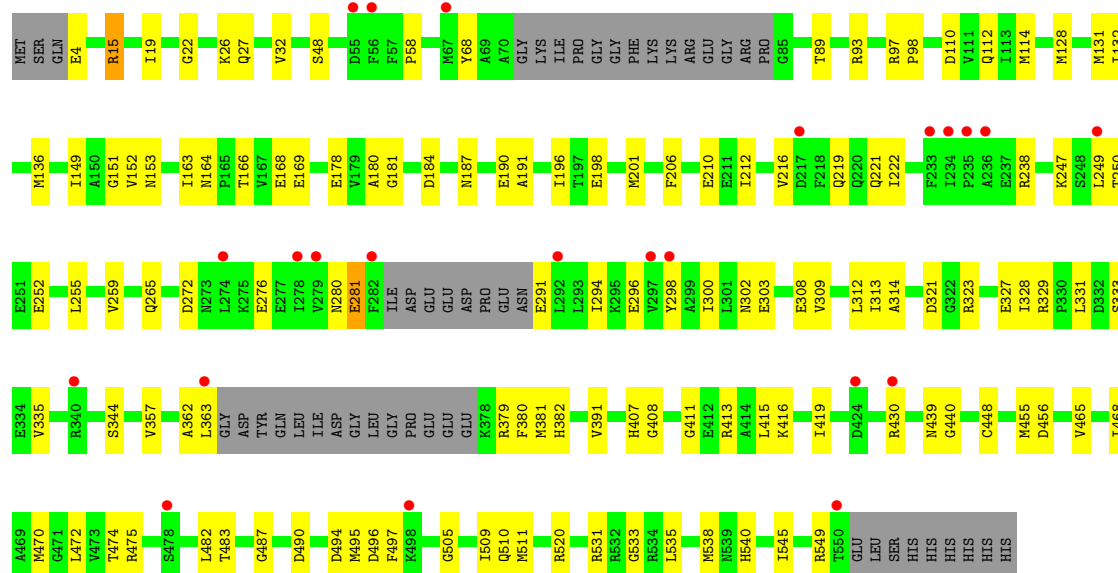


• Molecule 1: Polyribonucleotide nucleotidyltransferase

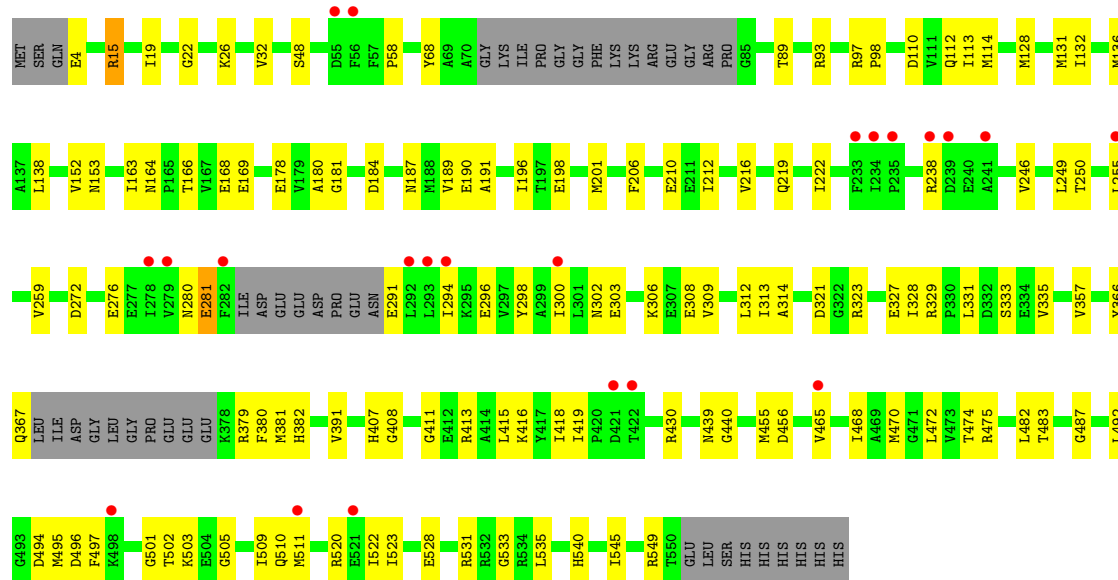




- Molecule 1: Polyribonucleotide nucleotidyltransferase



- Molecule 1: Polyribonucleotide nucleotidyltransferase



- Molecule 1: Polyribonucleotide nucleotidyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.70Å 93.77Å 130.24Å 98.22° 95.34° 120.01°	Depositor
Resolution (Å)	49.24 – 2.20 49.24 – 2.20	Depositor EDS
% Data completeness (in resolution range)	84.0 (49.24-2.20) 84.0 (49.24-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.223 , 0.249 0.223 , 0.243	Depositor DCC
R_{free} test set	7966 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.085 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24313	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: PEG, PPV, GOL

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	0.81	1/4035 (0.0%)	0.93	4/5447 (0.1%)
1	B	0.81	1/4029 (0.0%)	0.91	5/5441 (0.1%)
1	C	0.80	2/4033 (0.0%)	0.91	5/5446 (0.1%)
1	D	0.79	2/4067 (0.0%)	0.93	5/5492 (0.1%)
1	E	0.76	0/4030	0.93	6/5441 (0.1%)
1	F	0.78	1/4046 (0.0%)	0.94	6/5462 (0.1%)
All	All	0.79	7/24240 (0.0%)	0.93	31/32729 (0.1%)

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
1	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	58	PRO	N-CD	9.37	1.60	1.47
1	B	58	PRO	N-CD	7.99	1.58	1.47
1	F	58	PRO	N-CD	7.18	1.57	1.47
1	D	58	PRO	N-CD	7.09	1.57	1.47
1	A	58	PRO	N-CD	5.67	1.55	1.47
1	C	465	VAL	C-O	-5.41	1.18	1.24
1	D	522	ILE	C-O	-5.34	1.18	1.24

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	523	ILE	N-CA-C	-18.17	94.55	111.45
1	D	523	ILE	N-CA-C	-11.34	99.82	110.82
1	E	523	ILE	N-CA-C	-10.38	100.75	110.82
1	A	222	ILE	N-CA-C	-8.37	102.66	110.53
1	D	222	ILE	N-CA-C	-8.11	102.91	110.53
1	B	222	ILE	N-CA-C	-8.04	102.97	110.53
1	C	222	ILE	N-CA-C	-7.76	103.23	110.53
1	F	222	ILE	N-CA-C	-7.76	103.23	110.53
1	E	222	ILE	N-CA-C	-7.44	103.54	110.53
1	E	522	ILE	N-CA-C	-6.78	103.87	110.72
1	F	281	GLU	N-CA-C	5.97	117.48	110.97
1	C	58	PRO	CA-N-CD	-5.92	103.71	112.00
1	B	281	GLU	N-CA-C	5.90	117.41	110.97
1	C	281	GLU	N-CA-C	5.88	117.38	110.97
1	A	281	GLU	N-CA-C	5.79	117.28	110.97
1	E	281	GLU	N-CA-C	5.62	117.09	110.97
1	D	184	ASP	N-CA-C	5.61	120.12	113.16
1	B	184	ASP	N-CA-C	5.59	120.09	113.16
1	D	281	GLU	N-CA-C	5.56	117.03	110.97
1	F	184	ASP	N-CA-C	5.54	120.03	113.16
1	D	505	GLY	N-CA-C	5.37	117.83	110.69
1	B	505	GLY	N-CA-C	5.36	117.82	110.69
1	E	505	GLY	N-CA-C	5.33	117.78	110.69
1	B	58	PRO	CA-N-CD	-5.32	104.56	112.00
1	C	505	GLY	N-CA-C	5.30	117.73	110.69
1	A	184	ASP	N-CA-C	5.29	119.72	113.16
1	E	184	ASP	N-CA-C	5.28	119.71	113.16
1	F	505	GLY	N-CA-C	5.27	117.70	110.69
1	A	505	GLY	N-CA-C	5.25	117.67	110.69
1	C	184	ASP	N-CA-C	5.17	119.57	113.16
1	F	179	VAL	CB-CA-C	-5.01	103.10	110.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ARG	Sidechain

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	3976	0	3991	106	0
1	B	3970	0	3982	103	0
1	C	3974	0	3985	103	1
1	D	4007	0	4009	97	1
1	E	3971	0	3981	96	0
1	F	3987	0	4001	102	0
2	A	7	0	10	0	0
2	B	7	0	10	0	0
2	C	7	0	10	0	0
2	D	7	0	10	0	0
2	E	7	0	10	0	0
2	F	7	0	10	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
4	A	18	0	0	7	0
4	B	18	0	0	7	0
4	C	18	0	0	6	0
4	D	18	0	0	5	0
4	E	18	0	0	6	0
4	F	18	0	0	5	0
5	A	29	0	0	1	0
5	B	17	0	0	2	0
5	C	44	0	0	6	0
5	D	42	0	0	3	0
5	E	51	0	0	1	0
5	F	59	0	0	9	0
All	All	24313	0	24057	607	1

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 13.

All (607) 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:531:ARG:O	1:C:535:LEU:HD13	1.39	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:VAL:O	1:E:250:THR:HG23	1.39	1.20
1:A:531:ARG:O	1:A:535:LEU:HD13	1.38	1.20
1:B:531:ARG:O	1:B:535:LEU:HD13	1.42	1.18
1:D:246:VAL:O	1:D:250:THR:HG23	1.43	1.15
1:C:531:ARG:O	1:C:535:LEU:CD1	1.98	1.11
1:A:276:GLU:O	1:A:280:ASN:ND2	1.91	1.04
1:D:276:GLU:O	1:D:280:ASN:ND2	1.90	1.04
1:E:276:GLU:O	1:E:280:ASN:ND2	1.90	1.04
1:F:276:GLU:O	1:F:280:ASN:ND2	1.90	1.04
1:B:531:ARG:O	1:B:535:LEU:CD1	2.04	1.04
1:C:276:GLU:O	1:C:280:ASN:ND2	1.91	1.04
1:B:276:GLU:O	1:B:280:ASN:ND2	1.90	1.04
1:C:210:GLU:OE2	5:C:701:HOH:O	1.79	0.99
4:C:603[A]:PPV:O32	4:C:603[A]:PPV:O11	1.82	0.96
1:F:531:ARG:O	1:F:535:LEU:HD13	1.66	0.95
1:A:531:ARG:O	1:A:535:LEU:CD1	2.13	0.95
1:C:238:ARG:NH2	1:C:303:GLU:HG3	1.82	0.94
1:E:238:ARG:NH2	1:E:303:GLU:HG3	1.82	0.94
1:F:238:ARG:NH2	1:F:303:GLU:HG3	1.82	0.94
1:A:238:ARG:NH2	1:A:303:GLU:HG3	1.82	0.93
1:B:238:ARG:NH2	1:B:303:GLU:HG3	1.82	0.92
1:D:238:ARG:NH2	1:D:303:GLU:HG3	1.83	0.92
1:A:97:ARG:NH1	1:A:190:GLU:OE1	2.06	0.89
1:E:389:PHE:HB2	5:F:701:HOH:O	1.72	0.88
1:C:238:ARG:HH22	1:C:303:GLU:HG3	1.39	0.88
1:F:46:THR:OG1	5:F:701:HOH:O	1.92	0.88
1:A:238:ARG:HH22	1:A:303:GLU:HG3	1.39	0.87
1:D:238:ARG:HH22	1:D:303:GLU:HG3	1.40	0.86
1:F:238:ARG:HH22	1:F:303:GLU:HG3	1.40	0.85
1:B:238:ARG:HH22	1:B:303:GLU:HG3	1.39	0.85
1:B:98:PRO:HG3	1:B:131:MET:HE1	1.59	0.84
1:D:98:PRO:HG3	1:D:131:MET:HE1	1.59	0.84
1:D:210:GLU:OE2	5:D:701:HOH:O	1.95	0.84
1:C:212:ILE:O	1:C:216:VAL:HG23	1.78	0.83
1:A:212:ILE:O	1:A:216:VAL:HG23	1.78	0.83
1:C:98:PRO:HG3	1:C:131:MET:HE1	1.60	0.83
1:A:98:PRO:HG3	1:A:131:MET:HE1	1.59	0.82
1:D:212:ILE:O	1:D:216:VAL:HG23	1.78	0.82
1:E:212:ILE:O	1:E:216:VAL:HG23	1.78	0.82
1:E:238:ARG:HH22	1:E:303:GLU:HG3	1.40	0.82
1:B:98:PRO:HG3	1:B:131:MET:CE	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:PRO:HG3	1:C:131:MET:CE	2.10	0.82
1:E:98:PRO:HG3	1:E:131:MET:HE1	1.60	0.81
1:F:212:ILE:O	1:F:216:VAL:HG23	1.78	0.81
1:D:98:PRO:HG3	1:D:131:MET:CE	2.10	0.81
1:E:98:PRO:HG3	1:E:131:MET:CE	2.10	0.81
1:B:212:ILE:O	1:B:216:VAL:HG23	1.79	0.81
1:A:210:GLU:OE2	5:A:701:HOH:O	1.98	0.81
1:F:98:PRO:HG3	1:F:131:MET:HE1	1.60	0.81
4:F:603[A]:PPV:O32	4:F:603[A]:PPV:O11	1.97	0.80
1:D:97:ARG:NH1	1:D:190:GLU:OE1	2.14	0.80
1:A:98:PRO:HG3	1:A:131:MET:CE	2.10	0.80
1:F:98:PRO:HG3	1:F:131:MET:CE	2.10	0.80
4:A:603[A]:PPV:O32	4:A:603[A]:PPV:O11	1.98	0.79
1:E:531:ARG:O	1:E:535:LEU:HD23	1.83	0.78
1:B:210:GLU:OE2	5:B:701:HOH:O	2.01	0.78
1:C:97:ARG:NH1	1:C:190:GLU:OE1	2.18	0.77
1:E:210:GLU:OE2	5:E:701:HOH:O	2.01	0.77
4:A:603[B]:PPV:O31	4:A:603[B]:PPV:O32	2.03	0.76
1:C:247:LYS:C	1:C:250:THR:HG22	2.12	0.75
1:D:196:ILE:HD11	1:D:201:MET:HE2	1.70	0.74
1:F:196:ILE:HD11	1:F:201:MET:HE2	1.70	0.74
1:C:196:ILE:HD11	1:C:201:MET:HE2	1.71	0.73
1:F:448:CYS:SG	5:F:721:HOH:O	2.47	0.73
1:B:196:ILE:HD11	1:B:201:MET:HE2	1.71	0.72
1:F:210:GLU:OE2	5:F:702:HOH:O	2.06	0.72
1:D:128:MET:HE3	1:D:153:ASN:HB2	1.72	0.72
1:A:15:ARG:NH1	1:A:123:ASP:O	2.23	0.72
1:A:196:ILE:HD11	1:A:201:MET:HE2	1.70	0.72
1:C:448:CYS:SG	5:C:718:HOH:O	2.46	0.72
1:C:531:ARG:O	1:C:535:LEU:HD12	1.86	0.71
1:E:196:ILE:HD11	1:E:201:MET:HE2	1.70	0.71
1:A:4:GLU:O	1:A:4:GLU:HG2	1.89	0.71
1:C:247:LYS:HA	1:C:250:THR:CG2	2.21	0.70
1:B:247:LYS:C	1:B:250:THR:HG22	2.16	0.70
1:B:455:MET:HE3	1:B:545:ILE:HG23	1.73	0.70
1:F:97:ARG:NH1	1:F:190:GLU:OE1	2.25	0.70
1:D:455:MET:HE3	1:D:545:ILE:HG23	1.74	0.70
1:A:247:LYS:C	1:A:250:THR:HG22	2.17	0.69
1:A:455:MET:HE3	1:A:545:ILE:HG23	1.73	0.69
1:B:455:MET:CE	1:B:545:ILE:HG23	2.23	0.69
1:C:455:MET:HE3	1:C:545:ILE:HG23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:GLY:HA2	1:B:187:ASN:HB2	1.75	0.69
1:B:411:GLY:O	1:B:415:LEU:HD23	1.93	0.68
1:F:455:MET:HE3	1:F:545:ILE:HG23	1.73	0.68
1:F:455:MET:CE	1:F:545:ILE:HG23	2.23	0.68
1:D:411:GLY:O	1:D:415:LEU:HD23	1.94	0.68
1:D:455:MET:CE	1:D:545:ILE:HG23	2.24	0.68
1:F:411:GLY:O	1:F:415:LEU:HD23	1.94	0.68
1:A:455:MET:CE	1:A:545:ILE:HG23	2.23	0.68
1:B:531:ARG:O	1:B:535:LEU:HD12	1.94	0.68
1:D:465:VAL:HG22	1:D:502:THR:HG22	1.75	0.68
1:E:455:MET:CE	1:E:545:ILE:HG23	2.24	0.68
1:A:496:ASP:OD2	4:A:603[B]:PPV:O12	2.13	0.67
1:C:455:MET:CE	1:C:545:ILE:HG23	2.24	0.67
1:E:455:MET:HE3	1:E:545:ILE:HG23	1.74	0.67
1:E:181:GLY:HA2	1:E:187:ASN:HB2	1.77	0.67
1:A:128:MET:HE1	1:A:178:GLU:HG2	1.76	0.67
1:B:472:LEU:CD1	1:B:474:THR:HG23	2.26	0.66
1:E:411:GLY:O	1:E:415:LEU:HD23	1.94	0.66
1:C:411:GLY:O	1:C:415:LEU:HD23	1.94	0.66
1:C:181:GLY:HA2	1:C:187:ASN:HB2	1.78	0.66
1:D:181:GLY:HA2	1:D:187:ASN:HB2	1.76	0.66
1:A:411:GLY:O	1:A:415:LEU:HD23	1.94	0.66
1:B:128:MET:HE1	1:B:178:GLU:HG2	1.78	0.66
1:A:19:ILE:HD13	1:A:136:MET:HG3	1.78	0.66
1:A:472:LEU:CD1	1:A:474:THR:HG23	2.26	0.66
1:A:181:GLY:HA2	1:A:187:ASN:HB2	1.76	0.66
1:F:472:LEU:CD1	1:F:474:THR:HG23	2.26	0.66
1:C:472:LEU:CD1	1:C:474:THR:HG23	2.26	0.65
1:F:181:GLY:HA2	1:F:187:ASN:HB2	1.78	0.65
1:C:4:GLU:O	1:C:4:GLU:HG2	1.95	0.65
1:C:19:ILE:HD13	1:C:136:MET:HG3	1.78	0.65
1:E:472:LEU:CD1	1:E:474:THR:HG23	2.26	0.65
1:F:19:ILE:HD13	1:F:136:MET:HG3	1.79	0.65
1:F:472:LEU:HD11	1:F:474:THR:HG23	1.79	0.65
1:A:472:LEU:HD11	1:A:474:THR:HG23	1.79	0.64
1:B:19:ILE:HD13	1:B:136:MET:HG3	1.78	0.64
1:E:503:LYS:HG2	1:E:535:LEU:HD13	1.77	0.64
1:B:335:VAL:CG2	1:B:456:ASP:HB2	2.27	0.64
1:D:15:ARG:NH2	1:D:164:ASN:O	2.30	0.64
4:D:603[A]:PPV:O32	4:D:603[A]:PPV:O11	2.14	0.64
1:F:128:MET:HE3	1:F:153:ASN:HB2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:ILE:HD13	1:E:136:MET:HG3	1.79	0.64
1:E:335:VAL:CG2	1:E:456:ASP:HB2	2.28	0.64
1:D:335:VAL:CG2	1:D:456:ASP:HB2	2.28	0.64
1:D:472:LEU:CD1	1:D:474:THR:HG23	2.26	0.64
4:E:603[A]:PPV:O11	4:E:603[A]:PPV:O32	2.15	0.64
1:C:472:LEU:HD11	1:C:474:THR:HG23	1.79	0.64
1:B:472:LEU:HD11	1:B:474:THR:HG23	1.79	0.64
1:F:335:VAL:CG2	1:F:456:ASP:HB2	2.27	0.64
1:B:250:THR:OG1	1:B:255:LEU:HD12	1.98	0.64
1:D:19:ILE:HD13	1:D:136:MET:HG3	1.79	0.64
1:C:128:MET:HE1	1:C:178:GLU:HG2	1.80	0.63
1:E:472:LEU:HD11	1:E:474:THR:HG23	1.79	0.63
1:A:335:VAL:CG2	1:A:456:ASP:HB2	2.28	0.63
1:C:335:VAL:CG2	1:C:456:ASP:HB2	2.28	0.63
1:E:15:ARG:NH2	1:E:164:ASN:O	2.30	0.63
1:D:472:LEU:HD11	1:D:474:THR:HG23	1.79	0.63
1:E:128:MET:HE3	1:E:153:ASN:HB2	1.80	0.62
1:B:97:ARG:NH1	1:B:190:GLU:OE1	2.32	0.62
1:C:238:ARG:HB2	5:C:721:HOH:O	1.99	0.62
1:C:15:ARG:NH2	1:C:164:ASN:O	2.31	0.62
1:A:250:THR:OG1	1:A:255:LEU:HD12	1.98	0.62
1:F:191:ALA:O	1:F:413:ARG:NH1	2.33	0.61
4:C:603[B]:PPV:O31	4:C:603[B]:PPV:O32	2.17	0.61
1:A:191:ALA:O	1:A:413:ARG:NH1	2.33	0.61
1:C:247:LYS:HA	1:C:250:THR:HG22	1.82	0.61
1:E:456:ASP:OD1	1:E:549:ARG:NH1	2.34	0.61
1:C:381:MET:HE3	1:C:430:ARG:NE	2.16	0.61
1:B:191:ALA:O	1:B:413:ARG:NH1	2.34	0.61
1:B:523:ILE:HG22	1:B:523:ILE:O	2.01	0.61
1:C:191:ALA:O	1:C:413:ARG:NH1	2.33	0.61
1:F:381:MET:HE3	1:F:430:ARG:NE	2.16	0.61
1:D:191:ALA:O	1:D:413:ARG:NH1	2.34	0.60
1:D:381:MET:HE3	1:D:430:ARG:NE	2.16	0.60
1:E:97:ARG:NH1	1:E:190:GLU:OE1	2.34	0.60
1:E:191:ALA:O	1:E:413:ARG:NH1	2.34	0.60
1:D:291:GLU:OE1	5:D:702:HOH:O	2.16	0.60
1:E:497:PHE:CD1	1:E:511:MET:HB2	2.37	0.60
1:C:456:ASP:OD1	1:C:549:ARG:NH1	2.34	0.60
1:D:456:ASP:OD1	1:D:549:ARG:NH1	2.34	0.60
1:A:247:LYS:O	1:A:250:THR:HG22	2.01	0.60
1:C:247:LYS:CA	1:C:250:THR:HG22	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:SER:HB3	5:C:710:HOH:O	2.01	0.60
1:F:456:ASP:OD1	1:F:549:ARG:NH1	2.35	0.60
1:B:456:ASP:OD1	1:B:549:ARG:NH1	2.34	0.60
1:D:407:HIS:HE1	4:D:603[A]:PPV:O32	1.85	0.60
1:B:48:SER:HB3	1:B:110:ASP:HB2	1.84	0.60
1:E:48:SER:HB3	1:E:110:ASP:HB2	1.84	0.59
1:E:381:MET:HE3	1:E:430:ARG:NE	2.17	0.59
1:A:381:MET:HE3	1:A:430:ARG:NE	2.17	0.59
1:B:381:MET:HE3	1:B:430:ARG:NE	2.17	0.59
1:A:456:ASP:OD1	1:A:549:ARG:NH1	2.34	0.59
1:F:114:MET:HE3	5:F:745:HOH:O	2.02	0.59
1:C:48:SER:HB3	1:C:110:ASP:HB2	1.84	0.59
1:B:247:LYS:O	1:B:250:THR:HG22	2.03	0.59
1:D:48:SER:HB3	1:D:110:ASP:HB2	1.84	0.59
1:F:48:SER:HB3	1:F:110:ASP:HB2	1.84	0.59
1:B:391:VAL:HG12	1:B:391:VAL:O	2.02	0.59
1:C:391:VAL:HG12	1:C:391:VAL:O	2.03	0.58
1:E:298:TYR:O	1:E:302:ASN:ND2	2.34	0.58
1:D:391:VAL:HG12	1:D:391:VAL:O	2.02	0.58
1:B:329:ARG:HH22	1:B:440:GLY:HA3	1.68	0.58
1:D:465:VAL:HG13	1:D:501:GLY:O	2.02	0.58
1:C:329:ARG:HH22	1:C:440:GLY:HA3	1.69	0.58
1:D:465:VAL:HG13	1:D:501:GLY:C	2.29	0.58
1:C:298:TYR:O	1:C:302:ASN:ND2	2.35	0.58
4:B:603[A]:PPV:O32	4:B:603[A]:PPV:O11	2.21	0.58
1:D:329:ARG:HH22	1:D:440:GLY:HA3	1.69	0.58
1:E:391:VAL:HG12	1:E:391:VAL:O	2.03	0.58
1:F:391:VAL:HG12	1:F:391:VAL:O	2.02	0.58
1:B:407:HIS:HE1	4:B:603[A]:PPV:O32	1.86	0.57
1:D:298:TYR:O	1:D:302:ASN:ND2	2.34	0.57
1:F:528:GLU:OE2	1:F:531:ARG:NH1	2.38	0.57
1:A:48:SER:HB3	1:A:110:ASP:HB2	1.84	0.57
1:F:329:ARG:HH22	1:F:440:GLY:HA3	1.70	0.57
1:A:298:TYR:O	1:A:302:ASN:ND2	2.34	0.57
1:A:329:ARG:HH22	1:A:440:GLY:HA3	1.70	0.57
1:A:497:PHE:CD1	1:A:511:MET:HB2	2.38	0.57
1:C:309:VAL:O	1:C:313:ILE:HG13	2.05	0.57
1:D:309:VAL:O	1:D:313:ILE:HG13	2.05	0.57
1:F:15:ARG:NH2	1:F:164:ASN:O	2.37	0.57
1:F:309:VAL:O	1:F:313:ILE:HG13	2.05	0.57
1:B:309:VAL:O	1:B:313:ILE:HG13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:O	1:A:313:ILE:HG13	2.05	0.57
1:A:391:VAL:HG12	1:A:391:VAL:O	2.03	0.57
1:D:465:VAL:HG22	1:D:502:THR:CG2	2.35	0.57
1:C:98:PRO:HG3	1:C:131:MET:HE3	1.87	0.56
1:E:329:ARG:HH22	1:E:440:GLY:HA3	1.69	0.56
1:B:497:PHE:CD1	1:B:511:MET:HB2	2.40	0.56
1:D:407:HIS:CE1	4:D:603[A]:PPV:O32	2.58	0.56
1:A:407:HIS:HE1	4:A:603[A]:PPV:O32	1.87	0.56
1:A:98:PRO:HG3	1:A:131:MET:HE3	1.88	0.56
1:B:298:TYR:O	1:B:302:ASN:ND2	2.35	0.56
1:D:503:LYS:HG2	1:D:535:LEU:CD2	2.35	0.56
1:F:298:TYR:O	1:F:302:ASN:ND2	2.34	0.56
1:D:114:MET:HE3	5:D:736:HOH:O	2.06	0.56
1:E:309:VAL:O	1:E:313:ILE:HG13	2.05	0.56
1:E:497:PHE:HD1	1:E:511:MET:HB2	1.70	0.56
1:F:497:PHE:CD1	1:F:511:MET:HB2	2.41	0.56
1:F:335:VAL:HG23	1:F:456:ASP:HB2	1.87	0.56
1:D:189:VAL:HG22	1:D:511:MET:HE3	1.86	0.55
1:E:98:PRO:HG3	1:E:131:MET:HE3	1.87	0.55
1:F:98:PRO:HG3	1:F:131:MET:HE3	1.87	0.55
1:A:528:GLU:OE2	1:A:531:ARG:NH1	2.40	0.55
1:D:335:VAL:HG23	1:D:456:ASP:HB2	1.88	0.55
1:F:250:THR:OG1	1:F:255:LEU:HD12	2.06	0.55
1:E:335:VAL:HG23	1:E:456:ASP:HB2	1.87	0.55
1:A:335:VAL:HG23	1:A:456:ASP:HB2	1.87	0.55
1:E:246:VAL:O	1:E:250:THR:CG2	2.33	0.55
1:B:335:VAL:HG23	1:B:456:ASP:HB2	1.87	0.55
1:C:250:THR:OG1	1:C:255:LEU:HD12	2.07	0.55
1:D:98:PRO:HG3	1:D:131:MET:HE3	1.88	0.54
1:A:407:HIS:CE1	4:A:603[A]:PPV:O32	2.59	0.54
1:D:68:TYR:CD1	1:F:357:VAL:HG11	2.43	0.54
1:D:470:MET:HE3	1:D:482:LEU:O	2.07	0.54
1:A:97:ARG:NH1	1:A:190:GLU:CD	2.64	0.54
1:C:531:ARG:C	1:C:535:LEU:HD13	2.28	0.54
1:F:472:LEU:HD11	1:F:474:THR:CG2	2.37	0.54
1:C:247:LYS:HA	1:C:250:THR:HG21	1.88	0.54
1:C:335:VAL:HG23	1:C:456:ASP:HB2	1.88	0.54
1:C:472:LEU:HD11	1:C:474:THR:CG2	2.38	0.54
1:D:472:LEU:HD11	1:D:474:THR:CG2	2.38	0.54
1:E:472:LEU:HD11	1:E:474:THR:CG2	2.38	0.54
1:E:528:GLU:OE2	1:E:531:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:407:HIS:HE1	4:F:603[A]:PPV:O32	1.91	0.54
1:B:472:LEU:HD11	1:B:474:THR:CG2	2.37	0.54
1:E:407:HIS:HE1	4:E:603[A]:PPV:O32	1.90	0.54
1:B:15:ARG:NH1	1:B:164:ASN:O	2.41	0.53
1:C:344:SER:CB	5:C:710:HOH:O	2.56	0.53
1:C:470:MET:HE3	1:C:482:LEU:O	2.08	0.53
1:B:470:MET:HE3	1:B:482:LEU:O	2.09	0.53
1:D:465:VAL:CG2	1:D:502:THR:HG22	2.37	0.53
1:A:472:LEU:HD11	1:A:474:THR:CG2	2.38	0.53
1:B:98:PRO:HG3	1:B:131:MET:HE3	1.88	0.53
1:C:496:ASP:OD2	4:C:603[B]:PPV:O12	2.25	0.53
1:E:407:HIS:CE1	4:E:603[A]:PPV:O32	2.62	0.53
1:E:470:MET:HE3	1:E:482:LEU:O	2.08	0.53
1:E:503:LYS:HG2	1:E:535:LEU:CD1	2.38	0.53
1:C:497:PHE:CD1	1:C:511:MET:HB2	2.44	0.53
1:A:470:MET:HE3	1:A:482:LEU:O	2.08	0.52
1:D:497:PHE:CD1	1:D:511:MET:HB2	2.44	0.52
1:A:68:TYR:CD1	1:B:357:VAL:HG11	2.44	0.52
1:F:470:MET:HE3	1:F:482:LEU:O	2.08	0.52
1:A:490:ASP:OD2	4:A:603[B]:PPV:O12	2.27	0.52
1:B:407:HIS:CE1	4:B:603[A]:PPV:O32	2.63	0.52
1:B:523:ILE:O	1:B:523:ILE:CG2	2.57	0.52
1:B:128:MET:HG3	1:B:151:GLY:O	2.10	0.52
1:A:190:GLU:OE2	1:A:510:GLN:HG3	2.10	0.52
1:E:470:MET:HE1	1:E:483:THR:HA	1.92	0.52
4:F:603[B]:PPV:O32	4:F:603[B]:PPV:O21	2.28	0.51
1:B:528:GLU:OE2	1:B:531:ARG:NH1	2.44	0.51
1:F:470:MET:HE1	1:F:483:THR:HA	1.93	0.51
1:A:490:ASP:OD2	4:A:603[B]:PPV:P2	2.69	0.51
1:F:247:LYS:O	1:F:250:THR:HG22	2.11	0.51
1:A:470:MET:HE1	1:A:483:THR:HA	1.93	0.51
1:B:247:LYS:HA	1:B:250:THR:CG2	2.41	0.51
4:E:603[B]:PPV:O32	4:E:603[B]:PPV:O21	2.29	0.51
1:A:189:VAL:HG22	1:A:511:MET:HE3	1.93	0.50
1:D:470:MET:HE1	1:D:483:THR:HA	1.92	0.50
1:E:314:ALA:CB	1:E:475:ARG:HD2	2.41	0.50
1:D:314:ALA:CB	1:D:475:ARG:HD2	2.41	0.50
1:F:407:HIS:CE1	4:F:603[A]:PPV:O32	2.64	0.50
1:F:314:ALA:CB	1:F:475:ARG:HD2	2.42	0.50
1:A:128:MET:HG3	1:A:151:GLY:O	2.12	0.50
1:A:314:ALA:CB	1:A:475:ARG:HD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ALA:CB	1:B:475:ARG:HD2	2.41	0.50
1:D:528:GLU:OE2	1:D:531:ARG:NH1	2.45	0.50
1:F:198:GLU:OE2	1:F:198:GLU:N	2.40	0.50
1:B:247:LYS:HA	1:B:250:THR:HG22	1.93	0.49
1:B:470:MET:HE1	1:B:483:THR:HA	1.94	0.49
1:A:308:GLU:O	1:A:312:LEU:HD23	2.13	0.49
1:A:497:PHE:HD1	1:A:511:MET:HB2	1.77	0.49
1:B:333:SER:OG	1:B:540:HIS:HE1	1.96	0.49
1:D:366:TYR:O	1:D:367:GLN:C	2.55	0.49
1:C:314:ALA:CB	1:C:475:ARG:HD2	2.42	0.49
1:C:470:MET:HE1	1:C:483:THR:HA	1.93	0.49
1:E:490:ASP:OD2	4:E:603[B]:PPV:O12	2.30	0.49
1:A:357:VAL:HG11	1:C:68:TYR:CD1	2.47	0.49
4:D:603[B]:PPV:O32	4:D:603[B]:PPV:O21	2.31	0.49
1:F:308:GLU:O	1:F:312:LEU:HD23	2.13	0.49
1:A:247:LYS:HA	1:A:250:THR:HG22	1.95	0.49
1:B:308:GLU:O	1:B:312:LEU:HD23	2.13	0.48
1:F:291:GLU:HB3	1:F:294:ILE:HG12	1.95	0.48
1:F:486:GLN:CD	5:F:720:HOH:O	2.57	0.48
1:A:333:SER:OG	1:A:540:HIS:HE1	1.96	0.48
1:F:462:LYS:HD3	5:F:753:HOH:O	2.12	0.48
1:B:379:ARG:HD3	1:B:379:ARG:C	2.38	0.48
1:C:308:GLU:O	1:C:312:LEU:HD23	2.13	0.48
1:B:189:VAL:HG22	1:B:511:MET:HE3	1.95	0.48
1:C:407:HIS:HE1	4:C:603[A]:PPV:O32	1.95	0.48
1:E:308:GLU:O	1:E:312:LEU:HD23	2.13	0.48
1:E:328:ILE:HD11	1:E:533:GLY:HA2	1.95	0.48
1:A:291:GLU:HB3	1:A:294:ILE:HG12	1.96	0.48
1:C:128:MET:HG3	1:C:151:GLY:O	2.14	0.48
1:E:333:SER:OG	1:E:540:HIS:HE1	1.97	0.48
1:F:439:ASN:O	1:F:487:GLY:N	2.47	0.48
1:A:328:ILE:HD11	1:A:533:GLY:HA2	1.95	0.48
1:C:291:GLU:HB3	1:C:294:ILE:HG12	1.96	0.48
1:D:291:GLU:HB3	1:D:294:ILE:HG12	1.96	0.48
1:A:247:LYS:HA	1:A:250:THR:CG2	2.43	0.48
1:E:379:ARG:HD3	1:E:379:ARG:C	2.39	0.48
1:D:308:GLU:O	1:D:312:LEU:HD23	2.13	0.47
1:D:333:SER:OG	1:D:540:HIS:HE1	1.97	0.47
1:E:291:GLU:HB3	1:E:294:ILE:HG12	1.95	0.47
1:E:439:ASN:O	1:E:487:GLY:N	2.47	0.47
1:B:291:GLU:HB3	1:B:294:ILE:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:PHE:CG	1:B:419:ILE:HD13	2.49	0.47
1:C:439:ASN:O	1:C:487:GLY:N	2.47	0.47
1:C:490:ASP:OD2	4:C:603[B]:PPV:P2	2.73	0.47
1:E:470:MET:CE	1:E:483:THR:HA	2.44	0.47
1:B:439:ASN:O	1:B:487:GLY:N	2.47	0.47
1:D:190:GLU:OE2	1:D:510:GLN:NE2	2.48	0.47
1:C:333:SER:OG	1:C:540:HIS:HE1	1.97	0.47
1:D:328:ILE:HD11	1:D:533:GLY:HA2	1.96	0.47
1:D:470:MET:CE	1:D:483:THR:HA	2.45	0.47
1:E:199:GLN:O	1:E:203:GLU:CG	2.63	0.47
1:E:198:GLU:H	1:E:198:GLU:CD	2.22	0.47
1:B:68:TYR:CD1	1:C:357:VAL:HG11	2.50	0.47
1:C:131:MET:HE1	1:C:180:ALA:CB	2.45	0.47
1:D:439:ASN:O	1:D:487:GLY:N	2.46	0.47
1:F:333:SER:OG	1:F:540:HIS:HE1	1.97	0.47
1:F:497:PHE:HD1	1:F:511:MET:HB2	1.80	0.47
1:F:538:MET:HE1	5:F:741:HOH:O	2.13	0.47
1:A:19:ILE:HG23	1:A:32:VAL:HG13	1.97	0.47
1:A:439:ASN:O	1:A:487:GLY:N	2.48	0.47
1:B:523:ILE:O	1:B:527:LEU:HG	2.14	0.47
1:E:19:ILE:HG23	1:E:32:VAL:HG13	1.97	0.47
1:E:403:ARG:NH1	4:E:603[A]:PPV:O32	2.47	0.47
1:D:503:LYS:HG2	1:D:535:LEU:HD23	1.96	0.47
1:F:328:ILE:HD11	1:F:533:GLY:HA2	1.96	0.47
1:B:131:MET:HE1	1:B:180:ALA:CB	2.45	0.47
1:B:247:LYS:CA	1:B:250:THR:HG22	2.45	0.46
1:C:249:LEU:CD2	1:C:281:GLU:HG3	2.45	0.46
1:C:407:HIS:CE1	4:C:603[A]:PPV:O32	2.68	0.46
1:E:323:ARG:HB3	1:E:327:GLU:HG3	1.97	0.46
1:F:19:ILE:HG23	1:F:32:VAL:HG13	1.97	0.46
1:C:19:ILE:HG23	1:C:32:VAL:HG13	1.97	0.46
1:E:131:MET:HE1	1:E:180:ALA:CB	2.46	0.46
1:F:380:PHE:CG	1:F:419:ILE:HD13	2.50	0.46
1:F:470:MET:CE	1:F:483:THR:HA	2.46	0.46
1:B:328:ILE:HD11	1:B:533:GLY:HA2	1.96	0.46
1:C:323:ARG:HB3	1:C:327:GLU:HG3	1.97	0.46
1:E:198:GLU:CD	1:E:198:GLU:N	2.74	0.46
1:B:19:ILE:HG23	1:B:32:VAL:HG13	1.97	0.46
1:C:379:ARG:HD3	1:C:379:ARG:C	2.41	0.46
1:F:379:ARG:C	1:F:379:ARG:HD3	2.41	0.46
1:C:190:GLU:OE2	1:C:510:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:LEU:CD2	1:F:281:GLU:HG3	2.45	0.46
1:A:250:THR:OG1	1:A:255:LEU:CD1	2.64	0.46
1:C:329:ARG:O	1:C:331:LEU:HD13	2.16	0.46
1:A:131:MET:HE1	1:A:180:ALA:CB	2.46	0.46
1:A:472:LEU:HD12	1:A:494:ASP:HB2	1.98	0.46
1:D:246:VAL:O	1:D:250:THR:CG2	2.37	0.46
1:D:249:LEU:CD2	1:D:281:GLU:HG3	2.45	0.46
1:E:153:ASN:OD1	1:E:178:GLU:HG3	2.16	0.46
1:A:153:ASN:OD1	1:A:178:GLU:HG3	2.16	0.46
1:B:153:ASN:OD1	1:B:178:GLU:HG3	2.16	0.46
1:D:131:MET:HE1	1:D:180:ALA:CB	2.45	0.46
1:D:379:ARG:C	1:D:379:ARG:HD3	2.40	0.46
1:C:328:ILE:HD11	1:C:533:GLY:HA2	1.97	0.46
1:D:380:PHE:CG	1:D:419:ILE:HD13	2.51	0.46
1:E:249:LEU:CD2	1:E:281:GLU:HG3	2.46	0.46
1:A:470:MET:CE	1:A:483:THR:HA	2.45	0.46
1:B:250:THR:OG1	1:B:255:LEU:CD1	2.63	0.46
1:C:153:ASN:OD1	1:C:178:GLU:HG3	2.16	0.46
1:D:153:ASN:OD1	1:D:178:GLU:HG3	2.16	0.46
1:D:472:LEU:HD12	1:D:494:ASP:HB2	1.98	0.46
1:E:380:PHE:CG	1:E:419:ILE:HD13	2.51	0.46
1:F:153:ASN:OD1	1:F:178:GLU:HG3	2.16	0.46
1:B:468:ILE:HD11	1:B:483:THR:HG22	1.98	0.45
1:B:470:MET:CE	1:B:483:THR:HA	2.46	0.45
1:C:380:PHE:CG	1:C:419:ILE:HD13	2.51	0.45
1:C:470:MET:CE	1:C:483:THR:HA	2.46	0.45
1:E:329:ARG:O	1:E:331:LEU:HD13	2.16	0.45
1:A:329:ARG:O	1:A:331:LEU:HD13	2.16	0.45
1:B:323:ARG:HB3	1:B:327:GLU:HG3	1.98	0.45
1:B:329:ARG:O	1:B:331:LEU:HD13	2.15	0.45
1:B:472:LEU:HD12	1:B:494:ASP:HB2	1.98	0.45
1:D:503:LYS:HG2	1:D:535:LEU:HD21	1.98	0.45
1:E:472:LEU:HD12	1:E:494:ASP:HB2	1.98	0.45
1:F:472:LEU:HD12	1:F:494:ASP:HB2	1.98	0.45
1:C:472:LEU:HD12	1:C:494:ASP:HB2	1.99	0.45
1:F:131:MET:HE1	1:F:180:ALA:CB	2.46	0.45
1:A:249:LEU:CD2	1:A:281:GLU:HG3	2.46	0.45
1:B:249:LEU:CD2	1:B:281:GLU:HG3	2.46	0.45
1:F:323:ARG:HB3	1:F:327:GLU:HG3	1.97	0.45
1:B:132:ILE:HG13	1:B:219:GLN:NE2	2.32	0.45
1:C:538:MET:HE1	5:C:733:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ILE:HG23	1:D:32:VAL:HG13	1.98	0.45
1:F:179:VAL:HG12	1:F:180:ALA:N	2.31	0.45
1:F:329:ARG:O	1:F:331:LEU:HD13	2.17	0.45
1:F:534:ARG:HG3	1:F:535:LEU:HD12	1.98	0.45
1:A:380:PHE:CG	1:A:419:ILE:HD13	2.52	0.45
1:B:490:ASP:OD2	4:B:603[B]:PPV:P2	2.74	0.45
1:A:238:ARG:HH22	1:A:303:GLU:CG	2.21	0.45
1:D:314:ALA:HB3	1:D:475:ARG:HD2	1.99	0.45
1:D:323:ARG:HB3	1:D:327:GLU:HG3	1.98	0.45
1:E:238:ARG:HH21	1:E:303:GLU:HG3	1.77	0.45
1:A:314:ALA:HB3	1:A:475:ARG:HD2	1.99	0.45
1:A:379:ARG:HD3	1:A:379:ARG:C	2.41	0.45
1:E:22:GLY:O	1:E:26:LYS:HD3	2.17	0.45
1:A:190:GLU:OE2	1:A:510:GLN:NE2	2.50	0.45
1:E:468:ILE:HD11	1:E:483:THR:HG22	1.99	0.45
1:C:206:PHE:CE2	1:C:520:ARG:HG3	2.52	0.45
1:C:250:THR:OG1	1:C:255:LEU:CD1	2.65	0.45
1:E:357:VAL:HG11	1:F:68:TYR:CD1	2.52	0.45
1:B:314:ALA:HB3	1:B:475:ARG:HD2	1.99	0.44
1:F:465:VAL:HG22	1:F:502:THR:HG22	1.98	0.44
1:F:468:ILE:HD11	1:F:483:THR:HG22	1.98	0.44
1:B:112:GLN:NE2	1:B:114:MET:SD	2.91	0.44
1:C:112:GLN:NE2	1:C:114:MET:SD	2.91	0.44
1:E:112:GLN:NE2	1:E:114:MET:SD	2.91	0.44
1:A:206:PHE:CE2	1:A:520:ARG:HG3	2.52	0.44
1:B:538:MET:HE1	5:B:715:HOH:O	2.18	0.44
1:C:132:ILE:HG13	1:C:219:GLN:NE2	2.32	0.44
1:D:329:ARG:O	1:D:331:LEU:HD13	2.17	0.44
1:A:112:GLN:NE2	1:A:114:MET:SD	2.90	0.44
1:A:323:ARG:HB3	1:A:327:GLU:HG3	1.98	0.44
1:C:252:GLU:OE1	1:F:237:GLU:OE2	2.35	0.44
1:C:152:VAL:HG22	1:C:163:ILE:HG23	2.00	0.44
1:F:166:THR:OG1	1:F:169:GLU:HG3	2.18	0.44
1:A:166:THR:OG1	1:A:169:GLU:HG3	2.18	0.44
1:A:247:LYS:CA	1:A:250:THR:HG22	2.47	0.44
1:A:255:LEU:HD23	1:A:259:VAL:HG23	2.00	0.44
1:A:468:ILE:HD11	1:A:483:THR:HG22	1.98	0.44
1:B:321:ASP:OD2	1:B:323:ARG:CD	2.66	0.44
1:D:321:ASP:OD2	1:D:323:ARG:CD	2.66	0.44
1:F:314:ALA:HB3	1:F:475:ARG:HD2	2.00	0.44
1:D:166:THR:OG1	1:D:169:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:ALA:HB3	1:E:475:ARG:HD2	1.99	0.44
1:F:189:VAL:HG22	1:F:511:MET:HE3	1.99	0.44
1:B:152:VAL:HG22	1:B:163:ILE:HG23	2.00	0.44
1:B:206:PHE:CE2	1:B:520:ARG:HG3	2.53	0.44
1:D:112:GLN:NE2	1:D:114:MET:SD	2.91	0.44
1:F:112:GLN:NE2	1:F:114:MET:SD	2.91	0.44
1:B:22:GLY:O	1:B:26:LYS:HD3	2.18	0.44
1:D:22:GLY:O	1:D:26:LYS:HD3	2.18	0.44
1:D:468:ILE:HD11	1:D:483:THR:HG22	1.99	0.44
1:A:152:VAL:HG22	1:A:163:ILE:HG23	2.00	0.43
1:B:166:THR:OG1	1:B:169:GLU:HG3	2.18	0.43
1:F:255:LEU:HD23	1:F:259:VAL:HG23	2.00	0.43
1:C:22:GLY:O	1:C:26:LYS:HD3	2.18	0.43
1:E:132:ILE:HG13	1:E:219:GLN:NE2	2.33	0.43
1:E:152:VAL:HG22	1:E:163:ILE:HG23	2.00	0.43
1:F:22:GLY:O	1:F:26:LYS:HD3	2.18	0.43
1:F:362:ALA:O	1:F:363:LEU:CB	2.67	0.43
1:A:132:ILE:HG13	1:A:219:GLN:NE2	2.34	0.43
1:C:98:PRO:CG	1:C:131:MET:HE3	2.48	0.43
1:C:321:ASP:OD2	1:C:323:ARG:CD	2.66	0.43
1:C:468:ILE:HD11	1:C:483:THR:HG22	1.99	0.43
1:E:166:THR:OG1	1:E:169:GLU:HG3	2.18	0.43
1:F:152:VAL:HG22	1:F:163:ILE:HG23	2.00	0.43
1:F:206:PHE:CE2	1:F:520:ARG:HG3	2.53	0.43
1:A:321:ASP:OD2	1:A:323:ARG:CD	2.66	0.43
1:C:166:THR:OG1	1:C:169:GLU:HG3	2.18	0.43
1:C:247:LYS:O	1:C:250:THR:CG2	2.67	0.43
1:C:314:ALA:HB3	1:C:475:ARG:HD2	2.00	0.43
1:E:321:ASP:OD2	1:E:323:ARG:CD	2.66	0.43
1:C:89:THR:O	1:C:93:ARG:HG3	2.19	0.43
1:D:98:PRO:CG	1:D:131:MET:HE3	2.49	0.43
1:D:296:GLU:O	1:D:300:ILE:HG13	2.19	0.43
1:A:265:GLN:OE1	1:C:27:GLN:HG2	2.19	0.43
1:B:497:PHE:HD1	1:B:511:MET:HB2	1.78	0.43
1:C:32:VAL:HG21	1:C:136:MET:HB3	2.01	0.43
1:F:198:GLU:H	1:F:198:GLU:CD	2.26	0.43
1:F:475:ARG:HB2	1:F:477:ASP:OD1	2.18	0.43
1:F:496:ASP:OD2	4:F:603[B]:PPV:O22	2.36	0.43
1:E:98:PRO:CG	1:E:131:MET:HE3	2.48	0.43
1:F:132:ILE:HG13	1:F:219:GLN:NE2	2.33	0.43
1:F:296:GLU:O	1:F:300:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:HIS:HD2	1:A:408:GLY:O	2.02	0.43
1:B:496:ASP:OD2	4:B:603[B]:PPV:O12	2.37	0.43
1:C:272:ASP:O	1:C:276:GLU:HB2	2.19	0.43
1:D:32:VAL:HG21	1:D:136:MET:HB3	2.01	0.43
1:B:89:THR:O	1:B:93:ARG:HG3	2.19	0.43
1:B:272:ASP:O	1:B:276:GLU:HB2	2.19	0.43
1:C:238:ARG:HH22	1:C:303:GLU:CG	2.21	0.43
1:C:382:HIS:HD2	1:C:408:GLY:O	2.02	0.43
1:F:238:ARG:HH22	1:F:303:GLU:CG	2.22	0.43
1:A:22:GLY:O	1:A:26:LYS:HD3	2.19	0.43
1:A:98:PRO:CG	1:A:131:MET:HE3	2.48	0.43
1:B:509:ILE:HG22	1:B:510:GLN:N	2.34	0.43
1:C:296:GLU:O	1:C:300:ILE:HG13	2.19	0.43
1:D:152:VAL:HG22	1:D:163:ILE:HG23	2.01	0.43
1:F:32:VAL:HG21	1:F:136:MET:HB3	2.01	0.43
1:F:89:THR:O	1:F:93:ARG:HG3	2.19	0.43
1:F:198:GLU:N	1:F:198:GLU:CD	2.77	0.43
1:A:362:ALA:O	1:A:363:LEU:CB	2.67	0.42
1:C:149:ILE:HD12	1:C:149:ILE:C	2.45	0.42
1:D:382:HIS:HD2	1:D:408:GLY:O	2.02	0.42
1:E:472:LEU:HB2	1:E:495:MET:SD	2.59	0.42
1:A:272:ASP:O	1:A:276:GLU:HB2	2.19	0.42
1:A:296:GLU:O	1:A:300:ILE:HG13	2.20	0.42
1:B:98:PRO:CG	1:B:131:MET:HE3	2.49	0.42
1:D:132:ILE:HG13	1:D:219:GLN:NE2	2.33	0.42
1:D:472:LEU:HB2	1:D:495:MET:SD	2.60	0.42
1:E:265:GLN:OE1	1:F:27:GLN:HG2	2.20	0.42
1:F:321:ASP:OD2	1:F:323:ARG:CD	2.67	0.42
1:B:27:GLN:HG2	1:C:265:GLN:OE1	2.19	0.42
1:B:472:LEU:HB2	1:B:495:MET:SD	2.59	0.42
1:C:255:LEU:HD23	1:C:259:VAL:HG23	2.00	0.42
1:C:472:LEU:HB2	1:C:495:MET:SD	2.60	0.42
1:D:255:LEU:HD23	1:D:259:VAL:HG23	2.00	0.42
1:E:238:ARG:HH22	1:E:303:GLU:CG	2.21	0.42
1:E:255:LEU:HD23	1:E:259:VAL:HG23	2.00	0.42
1:E:362:ALA:O	1:E:363:LEU:CB	2.66	0.42
1:F:272:ASP:O	1:F:276:GLU:HB2	2.19	0.42
1:B:362:ALA:O	1:B:363:LEU:CB	2.67	0.42
1:D:198:GLU:N	1:D:198:GLU:CD	2.78	0.42
1:D:89:THR:O	1:D:93:ARG:HG3	2.19	0.42
1:D:206:PHE:CE2	1:D:520:ARG:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:ASP:OD2	1:D:323:ARG:HD2	2.20	0.42
1:E:206:PHE:CE2	1:E:520:ARG:HG3	2.55	0.42
1:A:32:VAL:HG21	1:A:136:MET:HB3	2.02	0.42
1:B:321:ASP:OD2	1:B:323:ARG:HD2	2.19	0.42
1:C:362:ALA:O	1:C:363:LEU:CB	2.67	0.42
1:E:89:THR:O	1:E:93:ARG:HG3	2.19	0.42
1:B:296:GLU:O	1:B:300:ILE:HG13	2.19	0.42
1:F:149:ILE:C	1:F:149:ILE:HD12	2.44	0.42
1:B:255:LEU:HD23	1:B:259:VAL:HG23	2.00	0.42
1:D:272:ASP:O	1:D:276:GLU:HB2	2.19	0.42
1:A:190:GLU:OE2	1:A:510:GLN:CG	2.68	0.42
1:A:519:THR:O	1:A:523:ILE:HG13	2.19	0.42
1:A:534:ARG:HG3	1:A:535:LEU:HD12	2.01	0.42
1:B:403:ARG:NH1	4:B:603[A]:PPV:O32	2.46	0.42
1:D:357:VAL:HG11	1:E:68:TYR:CD1	2.55	0.42
1:E:306:LYS:HA	1:E:492:LEU:HD13	2.02	0.42
1:A:306:LYS:HA	1:A:492:LEU:HD13	2.02	0.41
1:B:238:ARG:HH22	1:B:303:GLU:CG	2.21	0.41
1:D:509:ILE:HG22	1:D:510:GLN:N	2.35	0.41
1:F:321:ASP:OD2	1:F:323:ARG:HD2	2.20	0.41
1:B:32:VAL:HG21	1:B:136:MET:HB3	2.01	0.41
1:B:382:HIS:HD2	1:B:408:GLY:O	2.03	0.41
1:E:296:GLU:O	1:E:300:ILE:HG13	2.19	0.41
1:E:321:ASP:OD2	1:E:323:ARG:HD2	2.20	0.41
1:F:306:LYS:HA	1:F:492:LEU:HD13	2.02	0.41
1:F:382:HIS:HD2	1:F:408:GLY:O	2.03	0.41
1:F:472:LEU:HB2	1:F:495:MET:SD	2.60	0.41
1:A:238:ARG:HH21	1:A:303:GLU:HG3	1.77	0.41
1:A:472:LEU:HB2	1:A:495:MET:SD	2.60	0.41
1:E:32:VAL:HG21	1:E:136:MET:HB3	2.01	0.41
1:E:272:ASP:O	1:E:276:GLU:HB2	2.19	0.41
1:A:321:ASP:OD2	1:A:323:ARG:HD2	2.20	0.41
1:D:97:ARG:NH1	1:D:190:GLU:CD	2.77	0.41
1:A:89:THR:O	1:A:93:ARG:HG3	2.20	0.41
1:A:475:ARG:HB2	1:A:477:ASP:OD1	2.19	0.41
1:C:198:GLU:OE2	1:C:198:GLU:N	2.52	0.41
1:D:496:ASP:OD2	4:D:603[B]:PPV:O22	2.38	0.41
1:E:113:ILE:HD11	1:E:138:LEU:HD11	2.03	0.41
1:E:382:HIS:HD2	1:E:408:GLY:O	2.04	0.41
1:F:98:PRO:CG	1:F:131:MET:HE3	2.49	0.41
1:D:391:VAL:O	1:D:391:VAL:CG1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:ARG:O	1:E:331:LEU:CD1	2.69	0.41
1:F:4:GLU:O	1:F:22:GLY:C	2.64	0.41
1:B:149:ILE:C	1:B:149:ILE:HD12	2.45	0.41
1:B:418:ILE:C	1:B:418:ILE:HD12	2.46	0.41
1:B:531:ARG:C	1:B:535:LEU:HD13	2.34	0.41
1:D:113:ILE:HD11	1:D:138:LEU:HD11	2.02	0.41
1:E:391:VAL:O	1:E:391:VAL:CG1	2.69	0.41
1:C:321:ASP:OD2	1:C:323:ARG:HD2	2.20	0.41
1:D:465:VAL:HG13	1:D:501:GLY:CA	2.51	0.41
1:F:391:VAL:O	1:F:391:VAL:CG1	2.69	0.41
1:A:391:VAL:O	1:A:391:VAL:CG1	2.69	0.40
1:A:509:ILE:HG22	1:A:510:GLN:N	2.36	0.40
1:B:329:ARG:O	1:B:331:LEU:CD1	2.68	0.40
1:C:509:ILE:HG22	1:C:510:GLN:N	2.36	0.40
1:D:306:LYS:HA	1:D:492:LEU:HD13	2.02	0.40
1:D:416:LYS:HA	1:D:419:ILE:HD12	2.04	0.40
1:E:509:ILE:HG22	1:E:510:GLN:N	2.35	0.40
1:F:509:ILE:HG22	1:F:510:GLN:N	2.37	0.40
1:A:113:ILE:HD11	1:A:138:LEU:HD11	2.03	0.40
1:A:329:ARG:O	1:A:331:LEU:CD1	2.69	0.40
1:A:418:ILE:HG12	1:A:465:VAL:CG2	2.51	0.40
1:E:416:LYS:HA	1:E:419:ILE:HD12	2.03	0.40
1:B:323:ARG:CZ	1:B:329:ARG:HG3	2.52	0.40
1:B:490:ASP:OD2	4:B:603[B]:PPV:O12	2.39	0.40
1:C:416:LYS:HA	1:C:419:ILE:HD12	2.03	0.40
1:D:418:ILE:HD12	1:D:418:ILE:C	2.46	0.40
1:F:418:ILE:HD12	1:F:418:ILE:C	2.46	0.40
1:F:512:ASP:HA	5:F:731:HOH:O	2.21	0.40
1:A:27:GLN:HG2	1:B:265:GLN:OE1	2.21	0.40
1:E:199:GLN:O	1:E:203:GLU:HG2	2.22	0.40
1:C:497:PHE:HD1	1:C:511:MET:HB2	1.86	0.40
1:E:418:ILE:HD12	1:E:418:ILE:C	2.46	0.40

All (1) 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:C:168:GLU:OE2	1:D:168:GLU:OE1[1_454]	1.70	0.50

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	503/559 (90%)	480 (95%)	23 (5%)	0	100	100
1	B	502/559 (90%)	478 (95%)	24 (5%)	0	100	100
1	C	503/559 (90%)	480 (95%)	23 (5%)	0	100	100
1	D	507/559 (91%)	484 (96%)	23 (4%)	0	100	100
1	E	503/559 (90%)	482 (96%)	21 (4%)	0	100	100
1	F	505/559 (90%)	483 (96%)	22 (4%)	0	100	100
All	All	3023/3354 (90%)	2887 (96%)	136 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	431/472 (91%)	430 (100%)	1 (0%)	87	94
1	B	431/472 (91%)	429 (100%)	2 (0%)	81	90
1	C	431/472 (91%)	429 (100%)	2 (0%)	81	90
1	D	434/472 (92%)	432 (100%)	2 (0%)	81	90
1	E	430/472 (91%)	428 (100%)	2 (0%)	81	90
1	F	432/472 (92%)	428 (99%)	4 (1%)	70	84
All	All	2589/2832 (91%)	2576 (100%)	13 (0%)	81	90

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	B	4	GLU
1	B	15	ARG
1	C	15	ARG
1	C	221	GLN
1	D	4	GLU
1	D	15	ARG
1	E	4	GLU
1	E	15	ARG
1	F	15	ARG
1	F	226	ILE
1	F	250	THR
1	F	550	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	182	HIS
1	A	220	GLN
1	A	280	ASN
1	A	382	HIS
1	A	407	HIS
1	A	529	GLN
1	A	540	HIS
1	B	23	GLN
1	B	199	GLN
1	B	280	ASN
1	B	382	HIS
1	B	407	HIS
1	B	529	GLN
1	B	540	HIS
1	C	23	GLN
1	C	115	ASN
1	C	182	HIS
1	C	220	GLN
1	C	280	ASN
1	C	382	HIS
1	C	407	HIS
1	C	510	GLN
1	C	529	GLN

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Mol	Chain	Res	Type
1	C	540	HIS
1	D	115	ASN
1	D	280	ASN
1	D	382	HIS
1	D	407	HIS
1	D	529	GLN
1	D	540	HIS
1	E	23	GLN
1	E	280	ASN
1	E	382	HIS
1	E	407	HIS
1	E	529	GLN
1	E	540	HIS
1	F	23	GLN
1	F	115	ASN
1	F	220	GLN
1	F	280	ASN
1	F	382	HIS
1	F	407	HIS
1	F	529	GLN
1	F	540	HIS

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](#)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEG	D	601	-	6,6,6	0.67	0	5,5,5	0.47	0
4	PPV	C	603[B]	-	6,8,8	1.71	1 (16%)	12,13,13	1.56	1 (8%)
4	PPV	F	603[A]	-	6,8,8	1.02	0	12,13,13	1.32	2 (16%)
4	PPV	E	603[A]	-	6,8,8	1.10	0	12,13,13	1.30	1 (8%)
2	PEG	F	601	-	6,6,6	0.63	0	5,5,5	0.29	0
3	GOL	A	602	-	5,5,5	0.37	0	5,5,5	0.27	0
2	PEG	E	601	-	6,6,6	0.65	0	5,5,5	0.38	0
4	PPV	B	603[B]	-	6,8,8	1.69	1 (16%)	12,13,13	1.49	1 (8%)
3	GOL	C	602	-	5,5,5	0.36	0	5,5,5	0.32	0
4	PPV	A	603[A]	-	6,8,8	1.67	1 (16%)	12,13,13	1.76	4 (33%)
2	PEG	B	601	-	6,6,6	0.58	0	5,5,5	0.31	0
3	GOL	D	602	-	5,5,5	0.32	0	5,5,5	0.50	0
4	PPV	D	603[A]	-	6,8,8	1.07	0	12,13,13	1.42	2 (16%)
4	PPV	F	603[B]	-	6,8,8	0.99	0	12,13,13	1.00	1 (8%)
4	PPV	E	603[B]	-	6,8,8	1.00	1 (16%)	12,13,13	1.12	1 (8%)
2	PEG	C	601	-	6,6,6	0.63	0	5,5,5	0.40	0
3	GOL	E	602	-	5,5,5	0.23	0	5,5,5	0.58	0
4	PPV	C	603[A]	-	6,8,8	1.64	1 (16%)	12,13,13	1.58	2 (16%)
3	GOL	B	602	-	5,5,5	0.24	0	5,5,5	0.42	0
4	PPV	A	603[B]	-	6,8,8	1.71	1 (16%)	12,13,13	1.64	1 (8%)
3	GOL	F	602	-	5,5,5	0.29	0	5,5,5	0.21	0
2	PEG	A	601	-	6,6,6	0.55	0	5,5,5	0.41	0
4	PPV	D	603[B]	-	6,8,8	0.99	0	12,13,13	1.10	1 (8%)
4	PPV	B	603[A]	-	6,8,8	1.64	1 (16%)	12,13,13	1.68	2 (16%)

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
2	PEG	D	601	-	-	3/4/4/4	-
4	PPV	C	603[B]	-	-	0/6/6/6	-
4	PPV	F	603[A]	-	-	3/6/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PPV	E	603[A]	-	-	2/6/6/6	-
2	PEG	F	601	-	-	1/4/4/4	-
3	GOL	A	602	-	-	0/4/4/4	-
2	PEG	E	601	-	-	3/4/4/4	-
4	PPV	B	603[B]	-	-	0/6/6/6	-
3	GOL	C	602	-	-	0/4/4/4	-
4	PPV	A	603[A]	-	-	3/6/6/6	-
2	PEG	B	601	-	-	3/4/4/4	-
3	GOL	D	602	-	-	0/4/4/4	-
4	PPV	D	603[A]	-	-	2/6/6/6	-
4	PPV	F	603[B]	-	-	0/6/6/6	-
4	PPV	E	603[B]	-	-	2/6/6/6	-
2	PEG	C	601	-	-	2/4/4/4	-
3	GOL	E	602	-	-	0/4/4/4	-
4	PPV	C	603[A]	-	-	3/6/6/6	-
3	GOL	B	602	-	-	0/4/4/4	-
4	PPV	A	603[B]	-	-	0/6/6/6	-
3	GOL	F	602	-	-	1/4/4/4	-
2	PEG	A	601	-	-	3/4/4/4	-
4	PPV	D	603[B]	-	-	0/6/6/6	-
4	PPV	B	603[A]	-	-	3/6/6/6	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603[B]	PPV	P1-O31	3.76	1.62	1.50
4	C	603[B]	PPV	P1-O31	3.72	1.62	1.50
4	A	603[B]	PPV	P1-O31	3.71	1.62	1.50
4	A	603[A]	PPV	P1-O31	3.65	1.61	1.50
4	B	603[A]	PPV	P1-O31	3.59	1.61	1.50
4	C	603[A]	PPV	P1-O31	3.59	1.61	1.50
4	E	603[B]	PPV	P1-O21	2.01	1.62	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603[B]	PPV	O21-P1-O11	3.65	121.49	107.80
4	A	603[B]	PPV	O21-P1-O11	3.62	121.38	107.80
4	B	603[B]	PPV	O21-P1-O11	3.31	120.20	107.80
4	C	603[A]	PPV	O21-P1-O11	3.21	119.84	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603[A]	PPV	O21-P1-O11	3.10	119.42	107.80
4	B	603[A]	PPV	O21-P1-O11	3.00	119.07	107.80
4	B	603[A]	PPV	O21-P1-OPP	2.91	114.39	104.64
4	A	603[A]	PPV	O32-P2-OPP	-2.87	95.00	104.64
4	D	603[A]	PPV	O32-P2-OPP	-2.83	95.15	104.64
4	E	603[B]	PPV	O11-P1-O31	2.65	121.18	110.83
4	D	603[B]	PPV	O11-P1-O31	2.65	121.14	110.83
4	E	603[A]	PPV	O11-P1-O31	2.57	120.83	110.83
4	A	603[A]	PPV	O21-P1-OPP	2.48	112.94	104.64
4	F	603[A]	PPV	O11-P1-O31	2.45	120.38	110.83
4	C	603[A]	PPV	O32-P2-OPP	-2.39	96.60	104.64
4	F	603[A]	PPV	O32-P2-OPP	-2.37	96.69	104.64
4	D	603[A]	PPV	O11-P1-O31	2.35	120.01	110.83
4	F	603[B]	PPV	O11-P1-O31	2.26	119.63	110.83
4	A	603[A]	PPV	O12-P2-OPP	2.14	111.80	104.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603[A]	PPV	P1-OPP-P2-O32
4	B	603[A]	PPV	P1-OPP-P2-O32
4	C	603[A]	PPV	P1-OPP-P2-O32
4	D	603[A]	PPV	P1-OPP-P2-O32
4	E	603[A]	PPV	P1-OPP-P2-O32
4	E	603[B]	PPV	P1-OPP-P2-O32
4	F	603[A]	PPV	P1-OPP-P2-O32
2	F	601	PEG	O2-C3-C4-O4
2	A	601	PEG	O2-C3-C4-O4
2	E	601	PEG	O2-C3-C4-O4
2	B	601	PEG	O2-C3-C4-O4
2	C	601	PEG	O2-C3-C4-O4
2	D	601	PEG	O2-C3-C4-O4
2	D	601	PEG	O1-C1-C2-O2
2	A	601	PEG	C1-C2-O2-C3
2	B	601	PEG	C1-C2-O2-C3
2	A	601	PEG	O1-C1-C2-O2
2	E	601	PEG	C1-C2-O2-C3
2	C	601	PEG	C1-C2-O2-C3
4	C	603[A]	PPV	P1-OPP-P2-O22
3	F	602	GOL	O1-C1-C2-O2
2	D	601	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
2	B	601	PEG	O1-C1-C2-O2
4	A	603[A]	PPV	P1-OPP-P2-O22
4	B	603[A]	PPV	P1-OPP-P2-O22
4	D	603[A]	PPV	P1-OPP-P2-O22
4	E	603[A]	PPV	P1-OPP-P2-O22
4	E	603[B]	PPV	P1-OPP-P2-O22
4	F	603[A]	PPV	P1-OPP-P2-O22
4	A	603[A]	PPV	P1-OPP-P2-O12
4	B	603[A]	PPV	P1-OPP-P2-O12
4	C	603[A]	PPV	P1-OPP-P2-O12
4	F	603[A]	PPV	P1-OPP-P2-O12
2	E	601	PEG	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	603[B]	PPV	3	0
4	F	603[A]	PPV	3	0
4	E	603[A]	PPV	4	0
4	B	603[B]	PPV	3	0
4	A	603[A]	PPV	3	0
4	D	603[A]	PPV	3	0
4	F	603[B]	PPV	2	0
4	E	603[B]	PPV	2	0
4	C	603[A]	PPV	3	0
4	A	603[B]	PPV	4	0
4	D	603[B]	PPV	2	0
4	B	603[A]	PPV	4	0

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	511/559 (91%)	0.24	17 (3%)	49	46	19, 45, 87, 102	1 (0%)
1	B	510/559 (91%)	0.31	15 (2%)	53	50	17, 45, 87, 127	1 (0%)
1	C	511/559 (91%)	0.29	23 (4%)	38	35	19, 46, 92, 124	1 (0%)
1	D	515/559 (92%)	0.44	22 (4%)	40	36	21, 48, 105, 135	1 (0%)
1	E	511/559 (91%)	0.48	38 (7%)	20	18	19, 49, 107, 145	1 (0%)
1	F	513/559 (91%)	0.45	28 (5%)	30	27	21, 49, 102, 143	1 (0%)
All	All	3071/3354 (91%)	0.37	143 (4%)	36	33	17, 47, 97, 145	6 (0%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	498	LYS	5.2
1	D	293	LEU	5.1
1	F	293	LEU	5.0
1	C	282	PHE	4.8
1	F	498	LYS	4.6
1	A	55	ASP	4.6
1	E	293	LEU	4.5
1	F	282	PHE	4.2
1	F	239	ASP	3.8
1	E	241	ALA	3.8
1	B	424	ASP	3.8
1	E	424	ASP	3.7
1	E	282	PHE	3.7
1	E	498	LYS	3.7
1	D	241	ALA	3.7
1	F	252	GLU	3.6
1	B	54	GLY	3.6
1	F	292	LEU	3.6
1	C	498	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	55	ASP	3.5
1	D	279	VAL	3.5
1	A	71	GLY	3.5
1	F	238	ARG	3.4
1	F	241	ALA	3.4
1	E	235	PRO	3.4
1	E	294	ILE	3.3
1	E	234	ILE	3.3
1	F	279	VAL	3.3
1	B	363	LEU	3.3
1	E	363	LEU	3.3
1	F	71	GLY	3.2
1	E	292	LEU	3.2
1	A	234	ILE	3.2
1	D	234	ILE	3.2
1	B	282	PHE	3.2
1	E	278	ILE	3.2
1	B	498	LYS	3.2
1	E	236	ALA	3.1
1	D	235	PRO	3.1
1	F	234	ILE	3.1
1	F	55	ASP	3.1
1	A	282	PHE	3.0
1	A	498	LYS	3.0
1	F	4	GLU	3.0
1	C	274	LEU	2.9
1	B	233	PHE	2.9
1	F	278	ILE	2.9
1	B	235	PRO	2.9
1	A	236	ALA	2.8
1	E	56	PHE	2.8
1	E	279	VAL	2.8
1	B	234	ILE	2.8
1	C	430	ARG	2.8
1	C	56	PHE	2.8
1	D	278	ILE	2.8
1	E	249	LEU	2.8
1	E	71	GLY	2.7
1	C	298	TYR	2.7
1	A	233	PHE	2.7
1	A	250	THR	2.7
1	B	279	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	440	GLY	2.7
1	D	294	ILE	2.7
1	C	292	LEU	2.6
1	E	240	GLU	2.6
1	B	313	ILE	2.6
1	E	72	LYS	2.6
1	E	521	GLU	2.5
1	E	67	MET	2.5
1	C	279	VAL	2.5
1	F	294	ILE	2.5
1	E	242	LEU	2.5
1	B	274	LEU	2.5
1	D	292	LEU	2.5
1	E	421	ASP	2.5
1	A	235	PRO	2.5
1	B	278	ILE	2.5
1	C	278	ILE	2.5
1	E	339	PRO	2.4
1	F	240	GLU	2.4
1	C	234	ILE	2.4
1	D	56	PHE	2.4
1	D	282	PHE	2.4
1	F	243	VAL	2.4
1	A	274	LEU	2.4
1	E	239	ASP	2.4
1	F	362	ALA	2.4
1	F	550	THR	2.4
1	C	233	PHE	2.4
1	C	297	VAL	2.4
1	E	313	ILE	2.4
1	C	424	ASP	2.4
1	D	55	ASP	2.4
1	B	56	PHE	2.4
1	D	465	VAL	2.4
1	C	363	LEU	2.4
1	F	242	LEU	2.4
1	C	235	PRO	2.3
1	E	548	PRO	2.3
1	F	70	ALA	2.3
1	C	550	THR	2.3
1	D	233	PHE	2.3
1	D	300	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	249	LEU	2.3
1	E	238	ARG	2.3
1	E	243	VAL	2.3
1	F	246	VAL	2.3
1	B	421	ASP	2.3
1	F	235	PRO	2.3
1	C	340	ARG	2.3
1	E	233	PHE	2.2
1	E	379	ARG	2.2
1	C	67	MET	2.2
1	A	72	LYS	2.2
1	C	236	ALA	2.2
1	F	72	LYS	2.2
1	C	217	ASP	2.2
1	D	238	ARG	2.2
1	D	421	ASP	2.2
1	E	49	LYS	2.2
1	E	545	ILE	2.2
1	A	190	GLU	2.2
1	A	279	VAL	2.1
1	D	239	ASP	2.1
1	A	339	PRO	2.1
1	D	422	THR	2.1
1	A	340	ARG	2.1
1	A	292	LEU	2.1
1	E	300	ILE	2.1
1	F	233	PHE	2.1
1	E	458	GLY	2.1
1	C	478	SER	2.1
1	D	255	LEU	2.1
1	F	477	ASP	2.1
1	D	511	MET	2.0
1	D	521	GLU	2.0
1	A	278	ILE	2.0
1	F	54	GLY	2.0
1	E	4	GLU	2.0
1	B	362	ALA	2.0
1	F	236	ALA	2.0
1	E	529	GLN	2.0
1	E	304	LEU	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
3	GOL	E	602	6/6	0.75	0.16	57,60,63,68	0
4	PPV	B	603[A]	9/9	0.77	0.22	31,35,45,49	9
4	PPV	B	603[B]	9/9	0.77	0.22	46,51,62,62	9
4	PPV	D	603[A]	9/9	0.77	0.20	30,37,48,50	9
4	PPV	D	603[B]	9/9	0.77	0.20	56,60,66,69	9
4	PPV	C	603[A]	9/9	0.78	0.20	29,36,53,53	9
4	PPV	C	603[B]	9/9	0.78	0.20	49,54,62,63	9
4	PPV	A	603[A]	9/9	0.80	0.19	29,33,46,48	9
4	PPV	A	603[B]	9/9	0.80	0.19	43,51,60,61	9
3	GOL	C	602	6/6	0.81	0.16	47,48,52,54	0
3	GOL	B	602	6/6	0.81	0.14	52,55,56,59	0
3	GOL	F	602	6/6	0.84	0.11	57,59,60,60	0
2	PEG	E	601	7/7	0.85	0.16	54,58,61,62	0
2	PEG	D	601	7/7	0.86	0.12	52,53,57,58	0
3	GOL	A	602	6/6	0.86	0.11	53,56,59,62	0
4	PPV	F	603[A]	9/9	0.87	0.15	34,39,55,57	9
4	PPV	F	603[B]	9/9	0.87	0.15	53,61,68,70	9
2	PEG	F	601	7/7	0.88	0.14	51,56,59,61	0
2	PEG	B	601	7/7	0.88	0.11	52,53,55,56	0
4	PPV	E	603[A]	9/9	0.89	0.13	34,39,51,54	9
4	PPV	E	603[B]	9/9	0.89	0.13	58,63,68,68	9
2	PEG	C	601	7/7	0.89	0.12	47,52,55,55	0
3	GOL	D	602	6/6	0.89	0.10	55,57,60,61	0
2	PEG	A	601	7/7	0.90	0.11	48,49,53,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.