



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:07 PM UTC

PDB ID : 3L7I / pdb_00003l7i
Title : Structure of the Wall Teichoic Acid Polymerase TagF
Authors : Strynadka, N.C.J.; Lovering, A.L.
Deposited on : 2009-12-28
Resolution : 2.70 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

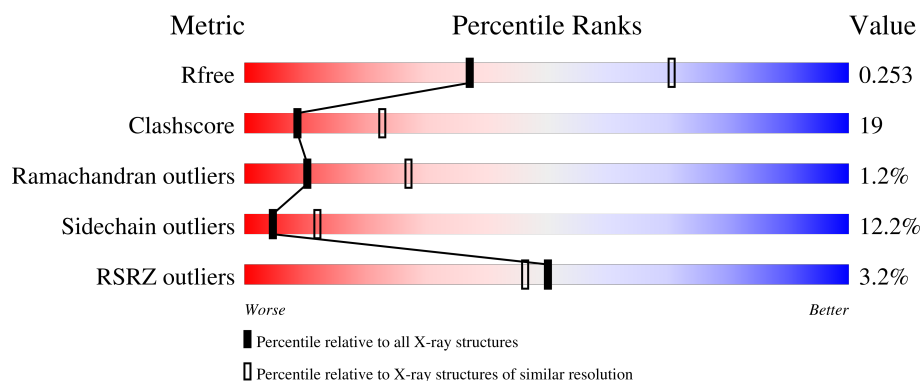
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	729	2% 34% 19% • 44%
1	B	729	2% 35% 17% • 44%
1	C	729	2% 35% 17% • 44%
1	D	729	2% 34% 17% 5% 44%

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	CL	B	733	-	-	X	-
3	CL	B	737	-	-	X	-
3	CL	D	734	-	-	X	-
4	EDO	D	732	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13962 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 Teichoic acid biosynthesis protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3469	2229	579	650	11			
1	B	411	Total	C	N	O	S	0	0	0
			3469	2229	579	650	11			
1	C	411	Total	C	N	O	S	0	0	0
			3469	2229	579	650	11			
1	D	408	Total	C	N	O	S	0	0	0
			3451	2218	576	646	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	722	LEU	-	expression tag	UNP Q5HLM5
A	723	GLU	-	expression tag	UNP Q5HLM5
A	724	HIS	-	expression tag	UNP Q5HLM5
A	725	HIS	-	expression tag	UNP Q5HLM5
A	726	HIS	-	expression tag	UNP Q5HLM5
A	727	HIS	-	expression tag	UNP Q5HLM5
A	728	HIS	-	expression tag	UNP Q5HLM5
A	729	HIS	-	expression tag	UNP Q5HLM5
B	722	LEU	-	expression tag	UNP Q5HLM5
B	723	GLU	-	expression tag	UNP Q5HLM5
B	724	HIS	-	expression tag	UNP Q5HLM5
B	725	HIS	-	expression tag	UNP Q5HLM5
B	726	HIS	-	expression tag	UNP Q5HLM5
B	727	HIS	-	expression tag	UNP Q5HLM5
B	728	HIS	-	expression tag	UNP Q5HLM5
B	729	HIS	-	expression tag	UNP Q5HLM5
C	722	LEU	-	expression tag	UNP Q5HLM5
C	723	GLU	-	expression tag	UNP Q5HLM5
C	724	HIS	-	expression tag	UNP Q5HLM5
C	725	HIS	-	expression tag	UNP Q5HLM5
C	726	HIS	-	expression tag	UNP Q5HLM5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	727	HIS	-	expression tag	UNP Q5HLM5
C	728	HIS	-	expression tag	UNP Q5HLM5
C	729	HIS	-	expression tag	UNP Q5HLM5
D	722	LEU	-	expression tag	UNP Q5HLM5
D	723	GLU	-	expression tag	UNP Q5HLM5
D	724	HIS	-	expression tag	UNP Q5HLM5
D	725	HIS	-	expression tag	UNP Q5HLM5
D	726	HIS	-	expression tag	UNP Q5HLM5
D	727	HIS	-	expression tag	UNP Q5HLM5
D	728	HIS	-	expression tag	UNP Q5HLM5
D	729	HIS	-	expression tag	UNP Q5HLM5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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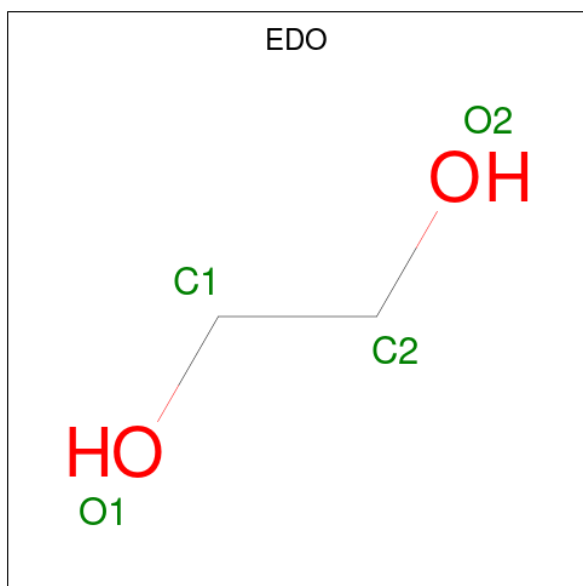
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	Cl	0	0
			12	12		
3	B	6	Total	Cl	0	0
			6	6		
3	C	5	Total	Cl	0	0
			5	5		
3	D	3	Total	Cl	0	0
			3	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

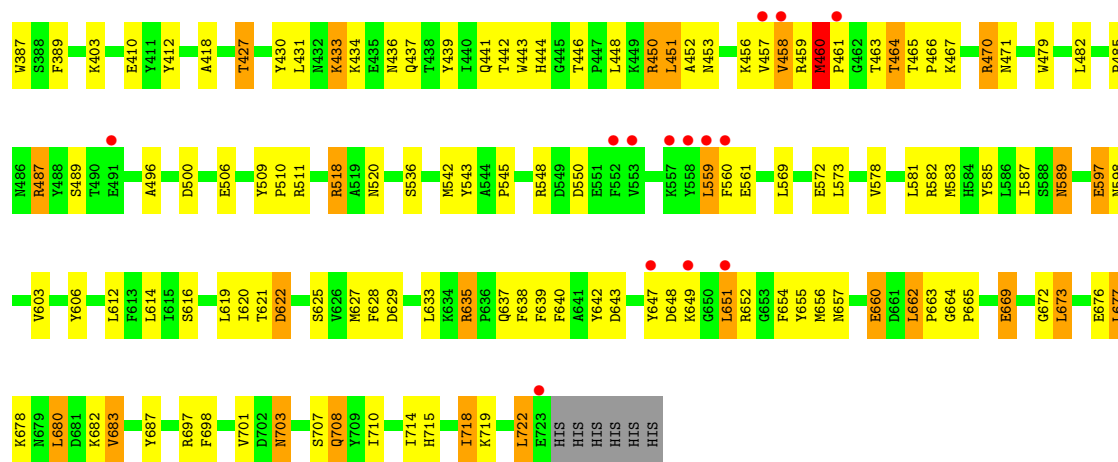
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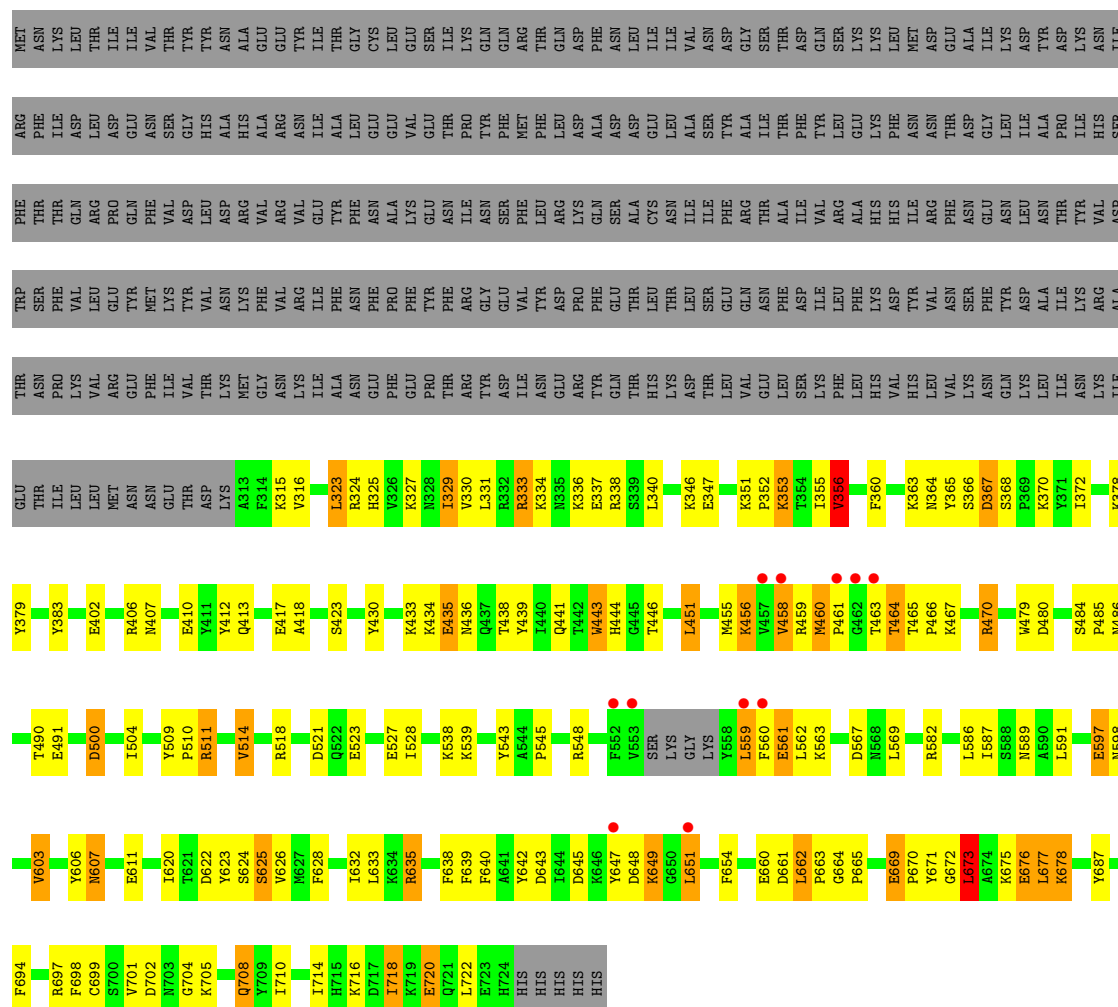
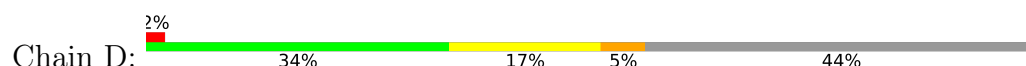
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	4	Total	O	0	0
			4	4		
5	C	5	Total	O	0	0
			5	5		
5	D	3	Total	O	0	0
			3	3		



• Molecule 1: Teichoic acid biosynthesis protein F



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	223.74Å 223.74Å 100.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.84 – 2.70 74.84 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (74.84-2.70) 97.9 (74.84-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.210 , 0.260 0.204 , 0.253	Depositor DCC
R_{free} test set	3483 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13962	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.73% 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: CL, EDO, SO4

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	0.62	0/3559	0.98	5/4809 (0.1%)
1	B	0.61	0/3559	0.95	4/4809 (0.1%)
1	C	0.56	0/3559	0.93	5/4809 (0.1%)
1	D	0.59	0/3541	0.94	10/4786 (0.2%)
All	All	0.59	0/14218	0.95	24/19213 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	366	SER	N-CA-C	7.48	119.07	108.74
1	C	366	SER	N-CA-C	6.41	116.91	107.88
1	C	316	VAL	N-CA-C	6.30	116.47	110.42
1	B	448	LEU	N-CA-C	-6.07	105.78	113.43
1	D	423	SER	N-CA-C	5.88	116.32	108.38
1	A	423	SER	N-CA-C	5.84	117.13	108.60
1	D	704	GLY	N-CA-C	-5.82	107.06	115.27
1	A	448	LEU	N-CA-C	-5.53	106.59	113.55
1	D	664	GLY	CA-C-N	5.52	125.99	120.14
1	D	664	GLY	C-N-CA	5.52	125.99	120.14
1	A	704	GLY	N-CA-C	-5.51	108.25	115.47
1	C	460	MET	CA-C-N	5.41	126.61	119.84
1	C	460	MET	C-N-CA	5.41	126.61	119.84
1	B	664	GLY	CA-C-N	5.36	125.11	119.76
1	B	664	GLY	C-N-CA	5.36	125.11	119.76
1	C	452	ALA	CB-CA-C	-5.33	110.41	116.54
1	D	661	ASP	N-CA-C	5.21	116.52	109.11
1	D	673	LEU	N-CA-C	-5.16	105.57	111.14
1	D	463	THR	N-CA-C	5.04	117.63	109.06
1	D	435	GLU	N-CA-C	-5.03	106.98	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	MET	CA-C-N	5.02	126.12	119.84
1	A	460	MET	C-N-CA	5.02	126.12	119.84
1	B	316	VAL	N-CA-C	5.02	115.74	110.62
1	D	356	VAL	N-CA-C	5.01	115.80	108.53

There are no chirality outliers.

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	3469	0	3375	125	0
1	B	3469	0	3375	132	0
1	C	3469	0	3375	136	0
1	D	3451	0	3347	127	0
2	A	15	0	0	1	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	12	0	0	2	0
3	B	6	0	0	5	0
3	C	5	0	0	1	0
3	D	3	0	0	4	0
4	B	4	0	6	2	0
4	C	8	0	12	0	0
4	D	8	0	12	4	0
5	A	6	0	0	0	0
5	B	4	0	0	1	0
5	C	5	0	0	0	0
5	D	3	0	0	0	0
All	All	13962	0	13502	512	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 19.

All (512) 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:B:563:LYS:H	1:B:563:LYS:HD2	1.07	1.19
1:D:383:TYR:CE2	1:D:718:ILE:HD11	1.92	1.04
1:B:470:ARG:HG2	1:B:470:ARG:HH11	1.20	1.02
1:D:333:ARG:HH11	1:D:333:ARG:HG2	1.25	0.97
1:A:648:ASP:HB2	1:A:651:LEU:HB2	1.42	0.97
1:B:382:ASN:N	1:B:382:ASN:HD22	1.62	0.92
1:B:346:LYS:HG3	1:B:349:ASN:ND2	1.85	0.91
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.32	0.90
1:C:648:ASP:HB2	1:C:651:LEU:HB3	1.54	0.89
1:D:353:LYS:HG3	3:D:734:CL:CL	2.09	0.89
1:B:563:LYS:HD2	1:B:563:LYS:N	1.88	0.88
1:C:383:TYR:CZ	1:C:718:ILE:HD11	2.09	0.88
1:C:383:TYR:CE2	1:C:718:ILE:HD11	2.10	0.86
1:A:458:VAL:HG13	1:A:460:MET:HE2	1.61	0.83
1:B:346:LYS:HG3	1:B:349:ASN:HD21	1.41	0.81
1:B:470:ARG:HG2	1:B:470:ARG:NH1	1.96	0.80
1:A:353:LYS:HG2	3:A:733:CL:CL	2.19	0.79
1:B:382:ASN:HD22	1:B:382:ASN:H	1.26	0.79
1:B:548:ARG:HD3	1:B:643:ASP:OD2	1.82	0.79
1:B:722:LEU:O	1:B:723:GLU:HG3	1.83	0.79
1:C:470:ARG:HH11	1:C:470:ARG:HG2	1.48	0.79
1:D:665:PRO:HG3	1:D:687:TYR:CZ	2.18	0.78
1:A:338:ARG:HD2	1:A:430:TYR:CD1	2.19	0.77
1:A:722:LEU:O	1:A:723:GLU:HG3	1.84	0.77
1:B:333:ARG:HH11	1:B:333:ARG:HG2	1.50	0.77
1:B:467:LYS:HE3	1:B:470:ARG:NH2	1.99	0.77
1:C:367:ASP:HB2	1:C:511:ARG:HD3	1.66	0.75
1:B:648:ASP:HB2	1:B:651:LEU:HB3	1.68	0.75
1:D:333:ARG:HH11	1:D:333:ARG:CG	1.98	0.75
1:A:648:ASP:CB	1:A:651:LEU:HB2	2.16	0.74
1:C:427:THR:HG23	1:C:439:TYR:OH	1.88	0.74
1:A:467:LYS:HE3	1:A:470:ARG:HH22	1.53	0.73
1:C:543:TYR:CZ	1:C:545:PRO:HG3	2.23	0.73
1:C:367:ASP:CG	1:C:368:SER:H	1.96	0.73
1:B:382:ASN:N	1:B:382:ASN:ND2	2.36	0.73
1:B:470:ARG:HH11	1:B:470:ARG:CG	2.00	0.72
1:C:542:MET:HE1	1:C:612:LEU:HB3	1.71	0.72
1:D:714:ILE:O	1:D:718:ILE:HG23	1.88	0.72
1:D:383:TYR:CZ	1:D:718:ILE:HD11	2.24	0.72
1:B:561:GLU:HB2	3:B:735:CL:CL	2.27	0.71
1:D:651:LEU:HD21	1:D:654:PHE:CD2	2.25	0.71
1:B:382:ASN:H	1:B:382:ASN:ND2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:662:LEU:HD23	1:D:662:LEU:H	1.55	0.71
1:C:620:ILE:HD13	1:C:673:LEU:HD11	1.73	0.71
1:D:464:THR:OG1	1:D:466:PRO:HD2	1.91	0.70
1:A:662:LEU:HD23	1:A:662:LEU:H	1.56	0.70
1:A:485:PRO:HG3	1:A:509:TYR:CE2	2.27	0.70
1:A:542:MET:HE1	1:A:613:PHE:CE1	2.26	0.70
1:D:324:ARG:HH11	4:D:732:EDO:H12	1.56	0.69
1:C:450:ARG:HA	1:C:655:TYR:CE2	2.27	0.69
1:C:648:ASP:HB2	1:C:651:LEU:CB	2.21	0.69
1:A:333:ARG:HH11	1:A:333:ARG:CG	2.06	0.69
1:B:663:PRO:HG3	1:B:694:PHE:CD2	2.28	0.68
1:B:542:MET:HE1	1:B:613:PHE:HD1	1.58	0.68
1:B:346:LYS:NZ	1:C:332:ARG:HH12	1.91	0.68
1:B:542:MET:HE1	1:B:613:PHE:CD1	2.28	0.68
1:C:347:GLU:HG3	1:C:436:ASN:HB2	1.74	0.68
1:A:338:ARG:HD3	1:A:412:TYR:OH	1.93	0.68
1:D:624:SER:OG	1:D:626:VAL:HG22	1.93	0.68
1:A:703:ASN:HB3	1:A:705:LYS:HB2	1.75	0.68
1:D:333:ARG:HG2	1:D:333:ARG:NH1	2.03	0.68
1:D:338:ARG:HD2	1:D:430:TYR:CD1	2.29	0.68
1:D:451:LEU:HD12	1:D:451:LEU:N	2.09	0.68
1:D:548:ARG:NH2	1:D:622:ASP:OD1	2.20	0.68
1:A:662:LEU:HB2	1:A:663:PRO:CD	2.24	0.67
1:B:443:TRP:HB3	5:B:741:HOH:O	1.94	0.67
1:C:714:ILE:O	1:C:718:ILE:HG23	1.94	0.67
1:B:543:TYR:CZ	1:B:545:PRO:HG3	2.29	0.67
1:C:451:LEU:H	1:C:451:LEU:HD12	1.59	0.67
1:B:624:SER:OG	1:B:626:VAL:HG22	1.93	0.67
1:D:543:TYR:CZ	1:D:545:PRO:HG3	2.30	0.67
1:C:665:PRO:HG3	1:C:687:TYR:CZ	2.30	0.67
1:C:446:THR:O	1:C:625:SER:HB2	1.95	0.67
1:C:458:VAL:HG13	1:C:460:MET:HE2	1.77	0.67
1:C:372:ILE:HD13	1:C:710:ILE:HG21	1.76	0.66
1:B:480:ASP:O	1:B:503:ARG:HG2	1.95	0.66
1:A:451:LEU:H	1:A:451:LEU:HD12	1.61	0.66
1:B:563:LYS:H	1:B:563:LYS:CD	1.93	0.66
1:C:542:MET:CE	1:C:612:LEU:HB3	2.25	0.66
1:A:662:LEU:HB2	1:A:663:PRO:HD3	1.76	0.66
1:B:383:TYR:CE2	1:B:718:ILE:HD11	2.31	0.66
1:B:338:ARG:HD2	1:B:430:TYR:CD1	2.31	0.66
1:B:648:ASP:HB2	1:B:651:LEU:CB	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:665:PRO:HG3	1:C:687:TYR:CE1	2.32	0.65
1:C:444:HIS:C	1:C:511:ARG:HH11	2.05	0.65
1:C:464:THR:OG1	1:C:466:PRO:HD2	1.96	0.65
1:C:703:ASN:ND2	1:C:703:ASN:H	1.94	0.65
1:D:365:TYR:CZ	1:D:370:LYS:HG3	2.32	0.65
1:C:375:TYR:CE1	1:C:708:GLN:HB2	2.31	0.65
1:B:513:ASP:HA	1:B:704:GLY:HA2	1.78	0.64
1:D:325:HIS:CE1	1:D:329:ILE:HD11	2.32	0.64
1:B:663:PRO:HG3	1:B:694:PHE:CG	2.32	0.64
1:C:511:ARG:HH22	1:C:629:ASP:CG	2.06	0.64
1:B:333:ARG:HH11	1:B:333:ARG:CG	2.11	0.64
1:B:353:LYS:HG3	3:B:733:CL:CL	2.35	0.63
1:A:467:LYS:HE3	1:A:470:ARG:NH2	2.12	0.63
1:C:382:ASN:H	1:C:382:ASN:ND2	1.95	0.63
1:A:548:ARG:HD3	1:A:643:ASP:OD2	1.98	0.63
1:A:583:MET:HE3	1:A:587:ILE:HG21	1.79	0.63
1:D:638:PHE:HE1	1:D:676:GLU:HG2	1.63	0.63
1:B:451:LEU:HD12	1:B:451:LEU:H	1.64	0.62
1:A:648:ASP:OD2	1:A:651:LEU:HD12	1.98	0.62
1:D:352:PRO:HD2	3:D:734:CL:CL	2.36	0.62
1:C:410:GLU:CD	1:C:410:GLU:H	2.08	0.62
1:C:545:PRO:HG2	1:C:583:MET:HE1	1.81	0.62
1:B:383:TYR:CE2	1:B:718:ILE:CD1	2.83	0.62
1:B:482:LEU:HD23	1:B:499:MET:HG3	1.81	0.62
1:A:641:ALA:HB1	1:A:644:ILE:HB	1.81	0.61
1:B:638:PHE:HE1	1:B:676:GLU:HG2	1.64	0.61
1:B:665:PRO:HG3	1:B:687:TYR:CZ	2.35	0.61
1:B:679:ASN:HD22	1:B:682:LYS:HE3	1.65	0.61
1:D:446:THR:O	1:D:625:SER:HB2	2.01	0.61
1:D:451:LEU:HD12	1:D:451:LEU:H	1.65	0.61
1:D:514:VAL:HG12	1:D:518:ARG:HG3	1.81	0.61
1:C:639:PHE:CE2	1:C:663:PRO:HD2	2.35	0.61
1:D:597:GLU:O	1:D:598:ASN:HB2	2.01	0.61
1:A:372:ILE:HD13	1:A:710:ILE:HG21	1.80	0.61
1:C:338:ARG:HD2	1:C:430:TYR:CD1	2.36	0.61
1:B:426:ARG:HD3	4:B:731:EDO:H22	1.81	0.60
1:D:607:ASN:H	1:D:607:ASN:ND2	1.99	0.60
1:D:372:ILE:HD13	1:D:710:ILE:HG21	1.83	0.60
1:D:338:ARG:HD3	1:D:412:TYR:OH	2.02	0.60
1:C:652:ARG:C	1:C:654:PHE:H	2.09	0.60
1:D:434:LYS:C	1:D:436:ASN:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:LEU:HD23	1:C:662:LEU:H	1.67	0.60
1:A:542:MET:HE1	1:A:613:PHE:CD1	2.37	0.59
1:D:633:LEU:HB3	1:D:635:ARG:HD3	1.84	0.59
1:A:669:GLU:HG2	1:A:671:TYR:H	1.67	0.59
1:C:633:LEU:HB3	1:C:635:ARG:HD3	1.84	0.59
1:C:458:VAL:HG13	1:C:460:MET:SD	2.43	0.59
1:D:347:GLU:HG3	1:D:436:ASN:HB2	1.85	0.59
1:A:480:ASP:O	1:A:503:ARG:HG2	2.03	0.58
1:D:458:VAL:HG12	1:D:460:MET:HB2	1.84	0.58
1:A:325:HIS:CE1	1:A:329:ILE:CD1	2.86	0.58
1:B:475:GLU:OE1	1:B:478:ARG:NH1	2.36	0.58
1:D:413:GLN:O	1:D:417:GLU:HG3	2.03	0.58
1:A:651:LEU:HD21	1:A:654:PHE:CD1	2.39	0.58
1:D:582:ARG:HD3	3:D:736:CL:CL	2.40	0.58
1:B:315:LYS:HB2	1:D:315:LYS:HD3	1.86	0.58
1:A:665:PRO:HG3	1:A:687:TYR:CZ	2.39	0.58
1:C:458:VAL:HG13	1:C:460:MET:CE	2.33	0.58
1:B:434:LYS:C	1:B:436:ASN:H	2.10	0.58
1:B:675:LYS:O	1:B:678:LYS:HB2	2.04	0.58
1:D:662:LEU:H	1:D:662:LEU:CD2	2.16	0.58
1:D:438:THR:HA	1:D:480:ASP:OD2	2.04	0.57
1:D:670:PRO:HD2	1:D:671:TYR:CD2	2.40	0.57
1:B:346:LYS:HZ1	1:C:332:ARG:HH12	1.52	0.57
1:C:459:ARG:O	1:C:459:ARG:HG3	2.04	0.57
1:D:325:HIS:CE1	1:D:329:ILE:CD1	2.88	0.56
1:D:465:THR:HB	1:D:466:PRO:HD3	1.87	0.56
1:A:451:LEU:HD12	1:A:451:LEU:N	2.19	0.56
1:B:607:ASN:OD1	1:B:607:ASN:N	2.34	0.56
1:B:620:ILE:HD11	1:B:677:LEU:HD21	1.87	0.56
1:B:662:LEU:H	1:B:662:LEU:HD23	1.71	0.56
1:A:458:VAL:CG1	1:A:460:MET:HE2	2.35	0.56
1:C:347:GLU:CG	1:C:436:ASN:HB2	2.35	0.56
1:C:367:ASP:CG	1:C:368:SER:N	2.61	0.56
1:D:355:ILE:HD13	1:D:714:ILE:HG21	1.87	0.56
1:B:347:GLU:O	1:B:436:ASN:ND2	2.39	0.56
1:B:652:ARG:C	1:B:654:PHE:H	2.11	0.56
1:C:458:VAL:HG12	1:C:458:VAL:O	2.05	0.56
1:A:420:HIS:CD2	1:A:438:THR:HB	2.40	0.56
1:A:624:SER:O	1:A:627:MET:HG2	2.05	0.56
1:C:338:ARG:HD3	1:C:412:TYR:OH	2.07	0.55
1:A:569:LEU:HD22	1:A:573:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LEU:HD23	1:B:327:LYS:HB2	1.87	0.55
1:D:640:PHE:CE2	1:D:642:TYR:HB3	2.41	0.55
1:C:585:TYR:O	1:C:589:ASN:OD1	2.25	0.55
1:A:352:PRO:O	1:A:718:ILE:HG21	2.06	0.55
1:A:652:ARG:C	1:A:654:PHE:H	2.14	0.55
1:A:485:PRO:HG3	1:A:509:TYR:CZ	2.41	0.55
1:B:559:LEU:HD13	1:B:559:LEU:O	2.06	0.55
1:D:324:ARG:NH1	4:D:732:EDO:H12	2.21	0.54
1:C:347:GLU:O	1:C:436:ASN:ND2	2.41	0.54
1:B:349:ASN:N	1:B:349:ASN:HD22	2.04	0.54
1:C:353:LYS:HG3	3:C:734:CL:CL	2.45	0.54
1:B:679:ASN:ND2	1:B:682:LYS:HB2	2.22	0.54
1:B:442:THR:HA	1:B:483:ILE:HG13	1.90	0.54
1:C:485:PRO:HD2	1:C:489:SER:HB2	1.88	0.54
1:D:485:PRO:HG3	1:D:509:TYR:CE2	2.43	0.54
1:A:313:ALA:HB2	3:A:743:CL:CL	2.45	0.54
1:C:470:ARG:HG2	1:C:470:ARG:NH1	2.15	0.54
1:B:338:ARG:HD3	1:B:412:TYR:OH	2.08	0.53
1:D:324:ARG:HD3	4:D:732:EDO:O1	2.09	0.53
1:A:569:LEU:CD2	1:A:573:LEU:HD12	2.38	0.53
1:D:490:THR:HG23	1:D:504:ILE:HD13	1.90	0.53
1:D:563:LYS:HD2	1:D:563:LYS:N	2.22	0.53
1:A:427:THR:HG23	1:A:439:TYR:OH	2.08	0.53
1:C:465:THR:HB	1:C:466:PRO:HD3	1.90	0.53
1:A:405:LYS:O	1:A:411:TYR:HB2	2.08	0.53
1:B:434:LYS:C	1:B:436:ASN:N	2.65	0.53
1:B:595:GLY:N	1:B:597:GLU:OE2	2.38	0.53
1:A:585:TYR:O	1:A:589:ASN:OD1	2.27	0.53
1:C:485:PRO:HG3	1:C:509:TYR:CE2	2.44	0.53
1:D:444:HIS:C	1:D:511:ARG:NH1	2.67	0.53
1:D:446:THR:HB	1:D:628:PHE:CD2	2.44	0.53
1:C:572:GLU:O	1:C:678:LYS:HE3	2.10	0.52
1:D:662:LEU:CD2	1:D:662:LEU:N	2.71	0.52
1:D:663:PRO:HG3	1:D:694:PHE:CG	2.44	0.52
1:B:511:ARG:HH22	1:B:629:ASP:CG	2.17	0.52
1:B:673:LEU:HD22	1:B:677:LEU:HD22	1.91	0.52
1:A:350:VAL:CG2	1:A:436:ASN:HD22	2.23	0.52
1:B:347:GLU:HG3	1:B:436:ASN:HB2	1.91	0.52
1:D:378:LYS:HD3	1:D:379:TYR:CE2	2.45	0.52
1:A:597:GLU:O	1:A:598:ASN:HB2	2.09	0.52
1:C:548:ARG:HD3	1:C:643:ASP:OD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:LYS:CE	1:C:470:ARG:HH22	2.23	0.52
1:D:697:ARG:HD3	1:D:698:PHE:CE2	2.45	0.52
1:A:662:LEU:HD23	1:A:662:LEU:N	2.22	0.52
1:B:325:HIS:CE1	1:B:329:ILE:HD13	2.44	0.52
1:C:662:LEU:H	1:C:662:LEU:CD2	2.23	0.52
1:A:351:LYS:HD2	1:A:417:GLU:OE1	2.10	0.52
1:C:597:GLU:O	1:C:598:ASN:HB2	2.10	0.52
1:D:356:VAL:HG22	1:D:418:ALA:CB	2.40	0.52
1:D:651:LEU:HD21	1:D:654:PHE:CE2	2.45	0.52
1:C:322:THR:O	1:C:326:VAL:HG23	2.11	0.51
1:B:662:LEU:H	1:B:662:LEU:CD2	2.23	0.51
1:C:673:LEU:HD22	1:C:677:LEU:HD22	1.91	0.51
1:A:514:VAL:HG12	1:A:518:ARG:HG3	1.92	0.51
1:D:470:ARG:HG2	1:D:470:ARG:HH11	1.74	0.51
1:D:669:GLU:OE2	1:D:672:GLY:N	2.43	0.51
1:A:481:TYR:CE2	1:A:713:LEU:HD21	2.45	0.51
1:D:439:TYR:N	1:D:480:ASP:OD2	2.33	0.51
1:B:378:LYS:HB3	1:B:379:TYR:CD2	2.46	0.51
1:B:380:TYR:HA	1:B:382:ASN:HD21	1.76	0.51
1:D:603:VAL:HG13	1:D:603:VAL:O	2.09	0.51
1:B:572:GLU:OE1	1:B:678:LYS:HE3	2.11	0.51
1:C:559:LEU:HD23	1:C:587:ILE:HG23	1.92	0.51
1:D:639:PHE:CZ	1:D:663:PRO:HD2	2.46	0.51
1:C:444:HIS:O	1:C:511:ARG:NH1	2.43	0.51
1:D:697:ARG:HD3	1:D:698:PHE:CZ	2.46	0.51
1:A:451:LEU:HA	1:A:455:MET:HE3	1.93	0.51
1:D:560:PHE:O	1:D:561:GLU:C	2.54	0.51
1:D:325:HIS:CE1	1:D:340:LEU:HB2	2.46	0.51
1:C:637:GLN:O	1:C:664:GLY:HA3	2.10	0.51
1:B:380:TYR:N	1:B:381:PRO:HD3	2.26	0.50
1:D:648:ASP:O	1:D:649:LYS:HB2	2.11	0.50
1:D:662:LEU:HB2	1:D:663:PRO:CD	2.41	0.50
1:D:368:SER:O	1:D:372:ILE:HG13	2.11	0.50
1:B:450:ARG:HA	1:B:655:TYR:CE2	2.47	0.50
1:C:451:LEU:HD12	1:C:451:LEU:N	2.26	0.50
1:A:470:ARG:HG2	1:A:470:ARG:HH11	1.77	0.50
1:C:434:LYS:C	1:C:436:ASN:H	2.18	0.50
1:C:657:ASN:ND2	1:C:660:GLU:OE1	2.44	0.50
1:C:662:LEU:HB2	1:C:663:PRO:HD3	1.94	0.50
1:B:646:LYS:O	1:B:648:ASP:N	2.41	0.50
1:A:662:LEU:N	1:A:662:LEU:CD2	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ASP:OD1	1:B:434:LYS:HE2	2.12	0.50
1:B:443:TRP:CD1	1:B:444:HIS:H	2.29	0.50
1:B:456:LYS:HA	1:B:456:LYS:HE2	1.93	0.50
1:A:344:THR:O	1:A:346:LYS:HG3	2.12	0.49
1:A:542:MET:HE1	1:A:613:PHE:HE1	1.76	0.49
1:B:443:TRP:CG	1:B:444:HIS:H	2.30	0.49
1:B:559:LEU:HD13	1:B:559:LEU:C	2.37	0.49
1:D:470:ARG:HG2	1:D:470:ARG:NH1	2.27	0.49
1:A:670:PRO:HG2	1:A:671:TYR:CE2	2.48	0.49
1:B:669:GLU:OE2	1:B:672:GLY:N	2.36	0.49
1:C:356:VAL:HG23	1:C:418:ALA:HB2	1.93	0.49
1:D:548:ARG:HD3	1:D:643:ASP:OD2	2.13	0.49
1:B:458:VAL:C	1:B:460:MET:H	2.20	0.49
1:C:639:PHE:CZ	1:C:663:PRO:HD2	2.47	0.49
1:D:329:ILE:HD12	1:D:336:LYS:HB2	1.95	0.49
1:B:378:LYS:HD3	1:B:379:TYR:CE2	2.47	0.49
1:D:451:LEU:HA	1:D:455:MET:HE3	1.94	0.49
1:B:350:VAL:HB	1:B:436:ASN:ND2	2.28	0.49
1:C:652:ARG:C	1:C:654:PHE:N	2.70	0.48
1:B:333:ARG:HG2	1:B:333:ARG:NH1	2.22	0.48
1:A:509:TYR:HB3	1:A:511:ARG:HG3	1.95	0.48
1:C:543:TYR:CE2	1:C:545:PRO:HG3	2.48	0.48
1:B:457:VAL:HG11	1:B:459:ARG:NH2	2.28	0.48
1:A:510:PRO:HA	1:A:706:ALA:HB3	1.94	0.48
1:C:487:ARG:HA	1:C:506:GLU:OE2	2.13	0.48
1:C:662:LEU:CD2	1:C:662:LEU:N	2.76	0.48
1:C:464:THR:HG23	1:C:467:LYS:CB	2.43	0.48
1:D:675:LYS:O	1:D:678:LYS:HB2	2.14	0.48
1:A:554:SER:O	1:A:555:LYS:HB2	2.13	0.48
1:A:572:GLU:O	1:A:678:LYS:HE3	2.13	0.48
1:C:550:ASP:OD1	1:C:550:ASP:C	2.56	0.48
1:C:703:ASN:H	1:C:703:ASN:HD22	1.60	0.48
1:D:456:LYS:HE2	1:D:456:LYS:HA	1.95	0.48
1:A:697:ARG:HD3	1:A:698:PHE:CZ	2.49	0.48
1:C:510:PRO:HB3	1:C:707:SER:OG	2.14	0.48
1:D:441:GLN:HG2	1:D:479:TRP:CE2	2.49	0.48
1:C:697:ARG:HD3	1:C:698:PHE:CE2	2.49	0.48
1:A:456:LYS:HE2	1:A:456:LYS:HA	1.95	0.48
1:A:679:ASN:ND2	1:A:682:LYS:HE3	2.29	0.47
1:B:380:TYR:C	1:B:382:ASN:ND2	2.72	0.47
1:B:540:VAL:HG22	1:B:578:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:621:THR:HG23	1:C:622:ASP:N	2.29	0.47
1:D:485:PRO:HG3	1:D:509:TYR:CZ	2.49	0.47
1:A:352:PRO:HA	1:A:419:SER:HB3	1.96	0.47
1:D:559:LEU:HD13	1:D:560:PHE:O	2.15	0.47
1:D:606:TYR:OH	1:D:611:GLU:OE1	2.31	0.47
1:A:543:TYR:CZ	1:A:545:PRO:HG3	2.49	0.47
1:A:638:PHE:HE1	1:A:676:GLU:HG2	1.78	0.47
1:B:347:GLU:CG	1:B:436:ASN:HB2	2.44	0.47
1:B:383:TYR:CE2	1:B:718:ILE:HD13	2.50	0.47
1:B:716:LYS:O	1:B:720:GLU:HG2	2.15	0.47
1:D:327:LYS:HZ1	4:D:732:EDO:H22	1.79	0.47
1:D:459:ARG:HG3	1:D:459:ARG:O	2.15	0.47
1:C:347:GLU:HA	1:C:434:LYS:HD3	1.95	0.47
1:D:451:LEU:N	1:D:451:LEU:CD1	2.76	0.47
1:A:333:ARG:HG2	1:A:333:ARG:NH1	2.12	0.47
1:A:387:TRP:HB3	1:A:389:PHE:CE2	2.50	0.47
1:C:441:GLN:O	1:C:482:LEU:HA	2.15	0.47
1:A:490:THR:HG23	1:A:504:ILE:HD13	1.97	0.46
1:B:446:THR:O	1:B:625:SER:HB2	2.14	0.46
1:C:442:THR:O	1:C:509:TYR:HE1	1.98	0.46
1:C:470:ARG:NH1	1:C:471:ASN:OD1	2.49	0.46
1:D:434:LYS:C	1:D:436:ASN:N	2.70	0.46
1:A:662:LEU:H	1:A:662:LEU:CD2	2.27	0.46
1:C:662:LEU:HB2	1:C:663:PRO:CD	2.45	0.46
1:C:680:LEU:HD23	1:C:680:LEU:HA	1.69	0.46
1:D:353:LYS:CG	3:D:734:CL:CL	2.91	0.46
1:B:351:LYS:HB3	3:B:733:CL:CL	2.52	0.46
1:B:403:LYS:HE3	3:B:737:CL:CL	2.52	0.46
1:C:382:ASN:ND2	1:C:382:ASN:N	2.62	0.46
1:C:597:GLU:H	1:C:597:GLU:HG2	1.15	0.46
1:D:559:LEU:HD12	1:D:559:LEU:O	2.15	0.46
1:B:384:ARG:NH2	1:B:417:GLU:OE1	2.49	0.46
1:C:582:ARG:NH2	1:C:606:TYR:O	2.48	0.46
1:D:485:PRO:HB2	1:D:486:ASN:ND2	2.31	0.46
1:A:561:GLU:H	1:A:561:GLU:HG2	1.55	0.46
1:C:433:LYS:HD2	1:C:439:TYR:HB2	1.98	0.46
1:B:387:TRP:HB3	1:B:389:PHE:CE2	2.50	0.46
1:A:470:ARG:HD2	1:A:474:ARG:HH21	1.81	0.45
1:B:458:VAL:HG12	1:B:460:MET:HB2	1.97	0.45
1:C:638:PHE:HE1	1:C:676:GLU:HG2	1.81	0.45
1:D:591:LEU:HA	1:D:591:LEU:HD23	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:673:LEU:HD22	1:D:677:LEU:HD22	1.98	0.45
1:A:345:ASP:OD2	1:A:434:LYS:HE3	2.16	0.45
1:C:316:VAL:HG13	1:C:317:ASN:N	2.30	0.45
1:D:360:PHE:HB2	1:D:363:LYS:HG2	1.97	0.45
1:B:583:MET:HE3	1:B:587:ILE:HD13	1.97	0.45
1:A:499:MET:HE3	1:A:499:MET:HB3	1.68	0.45
1:C:560:PHE:O	1:C:561:GLU:C	2.59	0.45
1:D:490:THR:HG23	1:D:504:ILE:HG21	1.99	0.45
1:A:651:LEU:HD23	1:A:651:LEU:O	2.16	0.45
1:C:378:LYS:HB3	1:C:379:TYR:CD2	2.52	0.45
1:D:367:ASP:HB2	1:D:511:ARG:CB	2.46	0.45
1:A:350:VAL:CG2	1:A:436:ASN:ND2	2.80	0.45
1:C:350:VAL:HG21	1:C:436:ASN:ND2	2.31	0.45
1:C:581:LEU:O	1:C:603:VAL:HG12	2.17	0.45
1:D:632:ILE:HG12	1:D:699:CYS:HB3	1.98	0.45
1:A:350:VAL:HG21	1:A:436:ASN:HD22	1.82	0.45
1:A:633:LEU:HB3	1:A:635:ARG:HD3	1.98	0.45
1:C:418:ALA:O	1:C:437:GLN:HG2	2.17	0.45
1:D:368:SER:OG	1:D:510:PRO:HD2	2.16	0.45
1:C:648:ASP:O	1:C:649:LYS:HB2	2.17	0.45
1:D:458:VAL:HG12	1:D:458:VAL:O	2.16	0.45
1:B:543:TYR:CE2	1:B:545:PRO:HG3	2.52	0.45
1:D:648:ASP:HB2	1:D:651:LEU:HB2	1.98	0.45
1:A:714:ILE:O	1:A:718:ILE:HG12	2.16	0.44
1:C:410:GLU:CD	1:C:410:GLU:N	2.74	0.44
1:A:627:MET:HE3	1:A:628:PHE:CZ	2.53	0.44
1:B:680:LEU:HA	1:B:680:LEU:HD23	1.78	0.44
1:C:559:LEU:HD12	1:C:559:LEU:O	2.17	0.44
1:C:441:GLN:HG2	1:C:479:TRP:CE2	2.52	0.44
1:B:456:LYS:HA	1:B:456:LYS:CE	2.48	0.44
1:B:721:GLN:C	1:B:723:GLU:H	2.25	0.44
1:C:559:LEU:CD1	1:C:559:LEU:C	2.91	0.44
1:C:638:PHE:CZ	1:C:683:VAL:HG11	2.53	0.44
1:A:406:ARG:O	1:A:407:ASN:HB2	2.16	0.44
1:A:443:TRP:CG	1:A:444:HIS:H	2.35	0.44
1:B:403:LYS:CE	3:B:737:CL:CL	3.03	0.44
1:C:434:LYS:C	1:C:436:ASN:N	2.76	0.44
1:D:665:PRO:HG3	1:D:687:TYR:OH	2.17	0.44
1:A:341:TYR:CD1	1:A:412:TYR:HB3	2.52	0.44
1:B:443:TRP:HH2	4:B:731:EDO:H11	1.82	0.44
1:C:316:VAL:HG23	1:D:331:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:627:MET:HE3	1:C:628:PHE:CZ	2.53	0.44
1:C:353:LYS:HB3	1:C:383:TYR:CD2	2.53	0.44
1:D:367:ASP:HB2	1:D:511:ARG:HD3	1.99	0.44
1:A:470:ARG:HG2	1:A:470:ARG:NH1	2.33	0.43
1:B:353:LYS:HA	1:B:718:ILE:HD12	2.00	0.43
1:B:648:ASP:O	1:B:649:LYS:HB2	2.16	0.43
1:D:347:GLU:O	1:D:436:ASN:ND2	2.51	0.43
1:D:410:GLU:OE1	1:D:410:GLU:N	2.42	0.43
1:D:523:GLU:O	1:D:527:GLU:HG3	2.18	0.43
1:D:699:CYS:C	1:D:701:VAL:H	2.26	0.43
1:A:350:VAL:HG21	1:A:436:ASN:ND2	2.33	0.43
1:A:350:VAL:HB	1:A:436:ASN:ND2	2.33	0.43
1:A:457:VAL:HG22	1:A:458:VAL:N	2.33	0.43
1:B:446:THR:HA	1:B:447:PRO:HD3	1.87	0.43
1:A:484:SER:HA	1:A:485:PRO:HD3	1.71	0.43
1:A:680:LEU:HD23	1:A:680:LEU:HA	1.80	0.43
1:C:387:TRP:HB3	1:C:389:PHE:CE2	2.53	0.43
2:A:731:SO4:O1	1:B:320:ARG:NH1	2.44	0.43
1:B:418:ALA:O	1:B:437:GLN:HG2	2.18	0.43
1:D:367:ASP:CG	1:D:368:SER:H	2.26	0.43
1:D:458:VAL:C	1:D:460:MET:HE2	2.43	0.43
1:A:333:ARG:CG	1:A:333:ARG:NH1	2.75	0.43
1:B:338:ARG:HD2	1:B:430:TYR:CG	2.54	0.43
1:B:372:ILE:HD13	1:B:710:ILE:HG21	2.00	0.43
1:C:542:MET:HE3	1:C:616:SER:OG	2.18	0.43
1:C:718:ILE:O	1:C:722:LEU:HD22	2.17	0.43
1:A:619:LEU:HB2	1:A:630:TYR:CD2	2.53	0.43
1:A:624:SER:OG	1:A:626:VAL:HG22	2.18	0.43
1:B:559:LEU:O	1:B:559:LEU:CD1	2.66	0.43
1:C:443:TRP:CG	1:C:444:HIS:H	2.36	0.43
1:C:448:LEU:HD13	1:C:627:MET:CE	2.48	0.43
1:D:562:LEU:HD11	1:D:591:LEU:HD11	1.99	0.43
1:B:484:SER:HA	1:B:485:PRO:HD3	1.68	0.43
1:B:554:SER:C	1:B:556:GLY:N	2.75	0.43
1:B:583:MET:HE2	1:B:587:ILE:HG21	2.00	0.43
1:C:715:HIS:NE2	1:C:719:LYS:HE3	2.34	0.43
1:D:363:LYS:HE2	1:D:364:ASN:OD1	2.19	0.43
1:D:539:LYS:HB2	1:D:539:LYS:HE3	1.85	0.43
1:C:327:LYS:O	1:C:331:LEU:HB2	2.19	0.43
1:C:569:LEU:HD22	1:C:573:LEU:HD12	1.99	0.43
1:D:528:ILE:HD13	1:D:611:GLU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:LEU:HA	1:C:323:LEU:HD12	1.68	0.42
1:D:383:TYR:CZ	1:D:718:ILE:CD1	2.99	0.42
1:D:662:LEU:HB2	1:D:663:PRO:HD3	2.01	0.42
1:C:542:MET:HE1	1:C:612:LEU:C	2.43	0.42
1:A:542:MET:HE3	1:A:542:MET:HB3	1.78	0.42
1:C:460:MET:HA	1:C:461:PRO:HD2	1.79	0.42
1:A:329:ILE:HG22	1:A:330:VAL:N	2.34	0.42
1:B:652:ARG:C	1:B:654:PHE:N	2.77	0.42
1:C:453:ASN:HB3	1:C:496:ALA:HA	2.01	0.42
1:D:464:THR:HG23	1:D:467:LYS:HB3	2.01	0.42
1:D:560:PHE:O	1:D:561:GLU:O	2.38	0.42
1:A:670:PRO:HG2	1:A:671:TYR:CD2	2.54	0.42
1:A:314:PHE:HB2	1:C:314:PHE:CZ	2.55	0.42
1:A:331:LEU:O	1:A:332:ARG:HB2	2.19	0.42
1:A:347:GLU:HG3	1:A:436:ASN:HB2	2.01	0.42
1:A:352:PRO:O	1:A:718:ILE:CG2	2.67	0.42
1:A:682:LYS:HE3	1:A:682:LYS:HB2	1.74	0.42
1:C:344:THR:O	1:C:346:LYS:HG3	2.19	0.42
1:C:364:ASN:HD22	1:C:366:SER:HB3	1.85	0.42
1:B:554:SER:C	1:B:556:GLY:H	2.27	0.42
1:B:651:LEU:O	1:B:651:LEU:HG	2.20	0.42
1:C:431:LEU:HD23	1:C:431:LEU:HA	1.65	0.42
1:C:439:TYR:CD1	1:C:439:TYR:C	2.97	0.42
1:C:614:LEU:HD23	1:C:614:LEU:HA	1.88	0.42
1:A:460:MET:HA	1:A:461:PRO:HD2	1.80	0.42
1:A:619:LEU:HB2	1:A:630:TYR:CE2	2.54	0.42
1:B:468:TYR:CD2	1:B:468:TYR:C	2.97	0.42
1:B:367:ASP:O	1:B:370:LYS:HB3	2.20	0.42
1:B:380:TYR:C	1:B:382:ASN:HD22	2.28	0.42
1:B:531:HIS:CD2	1:B:531:HIS:O	2.73	0.42
1:D:559:LEU:CD1	1:D:559:LEU:C	2.93	0.42
1:A:703:ASN:HB3	1:A:705:LYS:H	1.85	0.41
1:C:640:PHE:CE2	1:C:642:TYR:HB3	2.55	0.41
1:D:355:ILE:CD1	1:D:714:ILE:HG21	2.50	0.41
1:D:559:LEU:HD13	1:D:560:PHE:C	2.45	0.41
1:B:662:LEU:CD2	1:B:662:LEU:N	2.84	0.41
1:C:511:ARG:NH2	1:C:629:ASP:CG	2.77	0.41
1:C:518:ARG:C	1:C:520:ASN:H	2.28	0.41
1:D:367:ASP:O	1:D:370:LYS:HB3	2.21	0.41
1:D:443:TRP:CG	1:D:444:HIS:H	2.38	0.41
1:C:380:TYR:CE1	1:C:715:HIS:CE1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:697:ARG:HD3	1:C:698:PHE:CZ	2.54	0.41
1:C:701:VAL:O	1:C:701:VAL:HG12	2.20	0.41
1:D:500:ASP:OD1	1:D:500:ASP:N	2.50	0.41
1:A:446:THR:HB	1:A:628:PHE:CD2	2.55	0.41
1:B:532:LEU:HD21	1:B:606:TYR:CE2	2.56	0.41
1:B:697:ARG:HD3	1:B:698:PHE:CE2	2.55	0.41
1:A:434:LYS:HG3	1:A:437:GLN:OE1	2.20	0.41
1:A:585:TYR:CD1	1:A:585:TYR:C	2.98	0.41
1:A:708:GLN:HE21	1:A:708:GLN:HB2	1.61	0.41
1:B:439:TYR:C	1:B:439:TYR:CD1	2.97	0.41
1:B:515:LEU:HA	1:B:614:LEU:HD21	2.02	0.41
1:B:559:LEU:C	1:B:559:LEU:CD1	2.93	0.41
1:C:350:VAL:CG2	1:C:436:ASN:ND2	2.84	0.41
1:C:367:ASP:O	1:C:370:LYS:HB3	2.20	0.41
1:D:586:LEU:HA	1:D:586:LEU:HD23	1.45	0.41
1:A:378:LYS:HD3	1:A:379:TYR:CE2	2.55	0.41
1:A:509:TYR:HB3	1:A:511:ARG:CG	2.51	0.41
1:B:346:LYS:HZ3	1:C:332:ARG:HH12	1.67	0.41
1:A:439:TYR:CD1	1:A:439:TYR:C	2.99	0.41
1:A:578:VAL:HG22	1:A:599:PHE:O	2.20	0.41
1:D:705:LYS:O	1:D:708:GLN:HG2	2.21	0.41
1:A:470:ARG:NH1	1:A:474:ARG:NH2	2.69	0.41
1:A:677:LEU:O	1:A:678:LYS:C	2.64	0.41
1:D:716:LYS:O	1:D:720:GLU:HG2	2.20	0.41
1:A:458:VAL:O	1:A:458:VAL:HG12	2.21	0.41
1:A:485:PRO:HB2	1:A:486:ASN:ND2	2.35	0.41
1:A:651:LEU:HG	1:A:653:GLY:H	1.86	0.41
1:B:509:TYR:O	1:B:510:PRO:C	2.63	0.41
1:B:697:ARG:HD3	1:B:698:PHE:CZ	2.55	0.41
1:C:448:LEU:HD13	1:C:627:MET:HE1	2.03	0.41
1:A:534:LEU:HA	1:A:535:PRO:HD2	1.97	0.41
1:B:406:ARG:O	1:B:407:ASN:HB2	2.21	0.41
1:C:485:PRO:HG3	1:C:509:TYR:CZ	2.55	0.41
1:C:364:ASN:HD22	1:C:366:SER:CB	2.35	0.40
1:C:464:THR:HG23	1:C:467:LYS:HB3	2.03	0.40
1:D:467:LYS:CE	1:D:470:ARG:HH22	2.34	0.40
1:D:484:SER:HA	1:D:485:PRO:HD3	1.77	0.40
1:A:314:PHE:CE2	1:D:330:VAL:O	2.74	0.40
1:A:501:GLU:HA	1:A:504:ILE:HD12	2.02	0.40
1:A:554:SER:C	1:A:556:GLY:H	2.29	0.40
1:B:465:THR:N	1:B:466:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:VAL:CG1	1:C:317:ASN:N	2.83	0.40
1:C:669:GLU:OE2	1:C:672:GLY:N	2.54	0.40
1:D:347:GLU:CG	1:D:436:ASN:HB2	2.50	0.40
1:D:406:ARG:O	1:D:407:ASN:HB2	2.21	0.40
1:A:634:LYS:HE2	1:A:695:TYR:CE1	2.56	0.40
1:A:722:LEU:HA	1:A:722:LEU:HD12	1.76	0.40
1:B:351:LYS:HZ3	1:B:417:GLU:CD	2.30	0.40
1:B:358:GLU:O	1:B:423:SER:HB2	2.20	0.40
1:D:444:HIS:O	1:D:511:ARG:NH1	2.55	0.40
1:A:508:GLY:HA3	1:A:702:ASP:OD1	2.22	0.40
1:A:660:GLU:HB3	1:A:661:ASP:H	1.74	0.40
1:D:351:LYS:HE3	1:D:417:GLU:OE1	2.21	0.40
1:A:347:GLU:O	1:A:436:ASN:ND2	2.55	0.40
1:A:458:VAL:HG13	1:A:460:MET:CE	2.42	0.40
1:B:355:ILE:HG22	1:B:357:PHE:CE2	2.56	0.40
1:B:662:LEU:HB2	1:B:663:PRO:CD	2.51	0.40
1:B:720:GLU:HG2	1:B:720:GLU:H	1.62	0.40
1:D:323:LEU:HA	1:D:323:LEU:HD12	1.74	0.40
1:D:569:LEU:HD23	1:D:569:LEU:HA	1.85	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	409/729 (56%)	381 (93%)	23 (6%)	5 (1%)	10	27
1	B	409/729 (56%)	376 (92%)	29 (7%)	4 (1%)	12	32
1	C	409/729 (56%)	367 (90%)	39 (10%)	3 (1%)	18	41
1	D	404/729 (55%)	370 (92%)	26 (6%)	8 (2%)	6	16
All	All	1631/2916 (56%)	1494 (92%)	117 (7%)	20 (1%)	10	27

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	647	TYR
1	C	367	ASP
1	C	647	TYR
1	D	367	ASP
1	D	561	GLU
1	A	443	TRP
1	B	443	TRP
1	A	647	TYR
1	A	649	LYS
1	B	649	LYS
1	B	722	LEU
1	D	521	ASP
1	D	649	LYS
1	D	458	VAL
1	C	458	VAL
1	D	443	TRP
1	D	647	TYR
1	A	535	PRO
1	D	461	PRO
1	A	461	PRO

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	379/675 (56%)	333 (88%)	46 (12%)	5	12
1	B	379/675 (56%)	330 (87%)	49 (13%)	4	10
1	C	379/675 (56%)	337 (89%)	42 (11%)	6	15
1	D	377/675 (56%)	330 (88%)	47 (12%)	4	11
All	All	1514/2700 (56%)	1330 (88%)	184 (12%)	5	12

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	VAL
1	A	322	THR
1	A	323	LEU
1	A	329	ILE
1	A	333	ARG
1	A	356	VAL
1	A	388	SER
1	A	402	GLU
1	A	403	LYS
1	A	413	GLN
1	A	433	LYS
1	A	451	LEU
1	A	456	LYS
1	A	460	MET
1	A	486	ASN
1	A	487	ARG
1	A	491	GLU
1	A	502	GLU
1	A	506	GLU
1	A	511	ARG
1	A	514	VAL
1	A	538	LYS
1	A	542	MET
1	A	549	ASP
1	A	553	VAL
1	A	555	LYS
1	A	559	LEU
1	A	561	GLU
1	A	578	VAL
1	A	582	ARG
1	A	587	ILE
1	A	594	SER
1	A	597	GLU
1	A	607	ASN
1	A	610	SER
1	A	619	LEU
1	A	635	ARG
1	A	659	MET
1	A	660	GLU
1	A	662	LEU
1	A	669	GLU
1	A	673	LEU
1	A	677	LEU

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Mol	Chain	Res	Type
1	A	678	LYS
1	A	718	ILE
1	A	722	LEU
1	B	316	VAL
1	B	323	LEU
1	B	329	ILE
1	B	332	ARG
1	B	333	ARG
1	B	336	LYS
1	B	343	LEU
1	B	349	ASN
1	B	353	LYS
1	B	356	VAL
1	B	367	ASP
1	B	382	ASN
1	B	407	ASN
1	B	423	SER
1	B	433	LYS
1	B	438	THR
1	B	450	ARG
1	B	451	LEU
1	B	456	LYS
1	B	460	MET
1	B	470	ARG
1	B	483	ILE
1	B	491	GLU
1	B	511	ARG
1	B	514	VAL
1	B	555	LYS
1	B	559	LEU
1	B	563	LYS
1	B	578	VAL
1	B	594	SER
1	B	597	GLU
1	B	607	ASN
1	B	619	LEU
1	B	622	ASP
1	B	623	TYR
1	B	635	ARG
1	B	645	ASP
1	B	651	LEU
1	B	660	GLU

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Mol	Chain	Res	Type
1	B	661	ASP
1	B	662	LEU
1	B	669	GLU
1	B	673	LEU
1	B	677	LEU
1	B	678	LYS
1	B	702	ASP
1	B	703	ASN
1	B	718	ILE
1	B	722	LEU
1	C	315	LYS
1	C	332	ARG
1	C	348	ASP
1	C	353	LYS
1	C	367	ASP
1	C	382	ASN
1	C	403	LYS
1	C	427	THR
1	C	433	LYS
1	C	450	ARG
1	C	451	LEU
1	C	456	LYS
1	C	457	VAL
1	C	460	MET
1	C	463	THR
1	C	464	THR
1	C	470	ARG
1	C	487	ARG
1	C	500	ASP
1	C	518	ARG
1	C	536	SER
1	C	559	LEU
1	C	578	VAL
1	C	589	ASN
1	C	597	GLU
1	C	619	LEU
1	C	622	ASP
1	C	635	ARG
1	C	651	LEU
1	C	656	MET
1	C	660	GLU
1	C	662	LEU

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Mol	Chain	Res	Type
1	C	669	GLU
1	C	673	LEU
1	C	677	LEU
1	C	680	LEU
1	C	682	LYS
1	C	683	VAL
1	C	703	ASN
1	C	708	GLN
1	C	718	ILE
1	C	722	LEU
1	D	316	VAL
1	D	323	LEU
1	D	329	ILE
1	D	333	ARG
1	D	334	LYS
1	D	337	GLU
1	D	346	LYS
1	D	353	LYS
1	D	356	VAL
1	D	402	GLU
1	D	433	LYS
1	D	435	GLU
1	D	451	LEU
1	D	456	LYS
1	D	460	MET
1	D	464	THR
1	D	470	ARG
1	D	491	GLU
1	D	500	ASP
1	D	511	ARG
1	D	514	VAL
1	D	538	LYS
1	D	559	LEU
1	D	567	ASP
1	D	587	ILE
1	D	589	ASN
1	D	597	GLU
1	D	603	VAL
1	D	607	ASN
1	D	620	ILE
1	D	623	TYR
1	D	625	SER

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Mol	Chain	Res	Type
1	D	635	ARG
1	D	645	ASP
1	D	651	LEU
1	D	660	GLU
1	D	662	LEU
1	D	669	GLU
1	D	673	LEU
1	D	676	GLU
1	D	677	LEU
1	D	678	LYS
1	D	702	ASP
1	D	708	GLN
1	D	718	ILE
1	D	720	GLU
1	D	722	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	GLN
1	A	349	ASN
1	A	382	ASN
1	A	436	ASN
1	A	531	HIS
1	A	708	GLN
1	B	349	ASN
1	B	382	ASN
1	B	436	ASN
1	B	531	HIS
1	B	568	ASN
1	B	679	ASN
1	B	686	GLN
1	B	721	GLN
1	C	349	ASN
1	C	364	ASN
1	C	382	ASN
1	C	436	ASN
1	C	568	ASN
1	C	686	GLN
1	C	703	ASN
1	D	335	ASN
1	D	349	ASN

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Mol	Chain	Res	Type
1	D	413	GLN
1	D	436	ASN
1	D	517	ASN
1	D	531	HIS
1	D	607	ASN
1	D	703	ASN
1	D	708	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 26 are monoatomic - leaving 13 for Mogul analysis.

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	SO4	B	730	-	4,4,4	0.25	0	6,6,6	0.27	0
2	SO4	A	730	-	4,4,4	0.27	0	6,6,6	0.21	0
4	EDO	B	731	-	3,3,3	0.75	0	2,2,2	0.17	0
4	EDO	C	733	-	3,3,3	0.53	0	2,2,2	0.29	0
4	EDO	D	733	-	3,3,3	0.68	0	2,2,2	0.26	0
2	SO4	D	730	-	4,4,4	0.25	0	6,6,6	0.26	0
4	EDO	C	732	-	3,3,3	0.64	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	732	-	3,3,3	0.40	0	2,2,2	0.49	0
2	SO4	C	731	-	4,4,4	0.27	0	6,6,6	0.25	0
2	SO4	D	731	-	4,4,4	0.26	0	6,6,6	0.21	0
2	SO4	C	730	-	4,4,4	0.20	0	6,6,6	0.20	0
2	SO4	A	731	-	4,4,4	0.19	0	6,6,6	0.29	0
2	SO4	A	732	-	4,4,4	0.30	0	6,6,6	0.09	0

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
4	EDO	D	733	-	-	1/1/1/1	-
4	EDO	C	732	-	-	1/1/1/1	-
4	EDO	D	732	-	-	1/1/1/1	-
4	EDO	B	731	-	-	0/1/1/1	-
4	EDO	C	733	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	733	EDO	O1-C1-C2-O2
4	C	732	EDO	O1-C1-C2-O2
4	D	732	EDO	O1-C1-C2-O2
4	D	733	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	731	EDO	2	0
4	D	732	EDO	4	0
2	A	731	SO4	1	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	411/729 (56%)	0.08	11 (2%) 56 53	52, 67, 111, 170	0
1	B	411/729 (56%)	0.12	15 (3%) 46 42	55, 68, 125, 182	0
1	C	411/729 (56%)	0.14	15 (3%) 46 42	51, 73, 133, 181	0
1	D	408/729 (55%)	0.13	11 (2%) 56 53	55, 71, 129, 196	0
All	All	1641/2916 (56%)	0.12	52 (3%) 50 46	51, 70, 127, 196	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	560	PHE	5.7
1	D	651	LEU	5.1
1	B	560	PHE	4.8
1	D	553	VAL	4.5
1	B	462	GLY	4.1
1	A	313	ALA	4.1
1	B	553	VAL	3.8
1	C	461	PRO	3.7
1	A	553	VAL	3.6
1	C	651	LEU	3.6
1	B	651	LEU	3.5
1	B	558	TYR	3.4
1	C	647	TYR	3.4
1	A	558	TYR	3.3
1	A	560	PHE	3.3
1	D	457	VAL	3.2
1	B	559	LEU	3.2
1	D	458	VAL	3.1
1	D	552	PHE	3.1
1	A	647	TYR	3.0
1	C	560	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	649	LYS	2.8
1	D	647	TYR	2.6
1	D	462	GLY	2.6
1	C	457	VAL	2.6
1	B	332	ARG	2.6
1	C	559	LEU	2.4
1	D	559	LEU	2.4
1	B	556	GLY	2.4
1	A	461	PRO	2.4
1	D	461	PRO	2.3
1	A	462	GLY	2.3
1	D	463	THR	2.3
1	C	723	GLU	2.3
1	C	313	ALA	2.3
1	A	717	ASP	2.3
1	C	458	VAL	2.3
1	C	649	LYS	2.2
1	B	550	ASP	2.2
1	C	491	GLU	2.2
1	C	558	TYR	2.2
1	B	364	ASN	2.2
1	C	553	VAL	2.2
1	C	557	LYS	2.2
1	A	559	LEU	2.2
1	B	650	GLY	2.1
1	B	458	VAL	2.1
1	A	314	PHE	2.1
1	B	552	PHE	2.1
1	A	723	GLU	2.0
1	B	453	ASN	2.0
1	C	552	PHE	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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	C	731	5/5	0.70	0.12	116,116,116,116	0
4	EDO	C	733	4/4	0.73	0.13	77,77,77,77	0
2	SO4	D	731	5/5	0.79	0.13	113,113,113,113	0
4	EDO	C	732	4/4	0.84	0.14	58,58,58,58	0
2	SO4	B	730	5/5	0.84	0.10	100,100,100,100	0
4	EDO	B	731	4/4	0.87	0.14	53,53,53,53	0
3	CL	B	735	1/1	0.88	0.11	92,92,92,92	0
4	EDO	D	732	4/4	0.88	0.14	76,76,76,76	0
3	CL	A	744	1/1	0.89	0.10	88,88,88,88	0
3	CL	A	736	1/1	0.89	0.13	78,78,78,78	0
4	EDO	D	733	4/4	0.89	0.13	52,52,52,52	0
2	SO4	A	732	5/5	0.90	0.20	92,92,92,92	0
3	CL	A	734	1/1	0.92	0.09	84,84,84,84	0
3	CL	A	733	1/1	0.92	0.12	75,75,75,75	0
3	CL	C	737	1/1	0.92	0.17	80,80,80,80	0
3	CL	A	737	1/1	0.92	0.15	79,79,79,79	0
3	CL	D	734	1/1	0.93	0.08	71,71,71,71	0
3	CL	B	737	1/1	0.93	0.10	90,90,90,90	0
2	SO4	D	730	5/5	0.93	0.07	87,87,87,87	0
3	CL	B	734	1/1	0.94	0.06	83,83,83,83	0
2	SO4	A	731	5/5	0.94	0.12	78,78,78,78	0
3	CL	B	736	1/1	0.94	0.08	81,81,81,81	0
3	CL	A	742	1/1	0.94	0.09	85,85,85,85	0
2	SO4	C	730	5/5	0.94	0.07	95,95,95,95	0
3	CL	C	738	1/1	0.94	0.07	79,79,79,79	0
3	CL	A	741	1/1	0.95	0.08	73,73,73,73	0
3	CL	D	735	1/1	0.95	0.07	73,73,73,73	0
3	CL	D	736	1/1	0.95	0.07	80,80,80,80	0
3	CL	C	734	1/1	0.95	0.07	78,78,78,78	0
3	CL	C	735	1/1	0.96	0.07	78,78,78,78	0
3	CL	C	736	1/1	0.96	0.07	64,64,64,64	0
3	CL	A	743	1/1	0.96	0.15	74,74,74,74	0
2	SO4	A	730	5/5	0.96	0.10	76,76,76,76	0
3	CL	B	733	1/1	0.96	0.08	82,82,82,82	0
3	CL	A	739	1/1	0.96	0.08	61,61,61,61	0
3	CL	A	735	1/1	0.97	0.19	69,69,69,69	0
3	CL	A	740	1/1	0.97	0.11	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	738	1/1	0.97	0.10	72,72,72,72	0
3	CL	B	732	1/1	0.99	0.20	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.