



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:29 AM UTC

PDB ID : 1W8J / pdb_00001w8j
Title : Crystal Structure Of Myosin V Motor Domain - Nucleotide-Free
Authors : Coureux, P.-D.; Sweeney, H.L.; Houdusse, A.
Deposited on : 2004-09-22
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

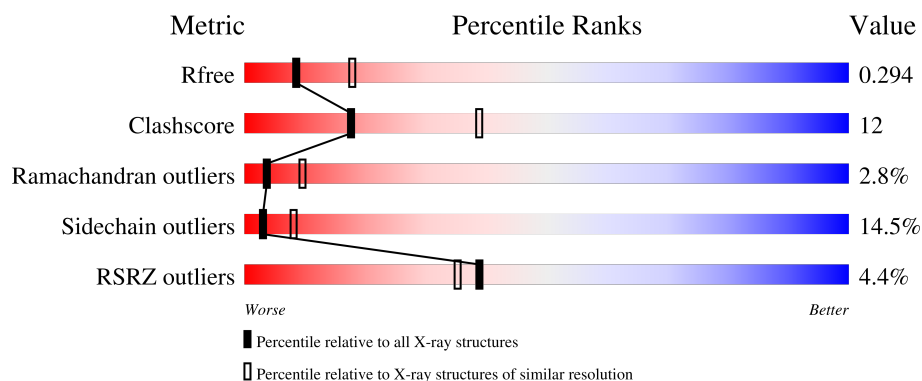
1 Overall quality at a glance

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	766	2% 64% 24% 5% • 6%
1	B	766	2% 64% 25% 5% 6%
1	C	766	5% 60% 28% 6% • 6%
1	D	766	7% 58% 28% 7% • 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 22756 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 MYOSIN VA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	722	Total	C	N	O	S	0	0	0
			5751	3685	972	1063	31			
1	B	719	Total	C	N	O	S	0	0	1
			5701	3652	954	1064	31			
1	C	723	Total	C	N	O	S	0	0	0
			5700	3651	964	1054	31			
1	D	717	Total	C	N	O	S	0	0	0
			5549	3535	948	1036	30			

- 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	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	5	Total	O	0	0
			5	5		
3	C	13	Total	O	0	0
			13	13		
3	D	4	Total	O	0	0
			4	4		

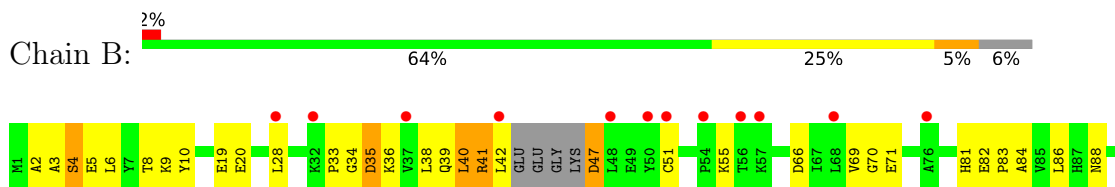
3 Residue-property plots

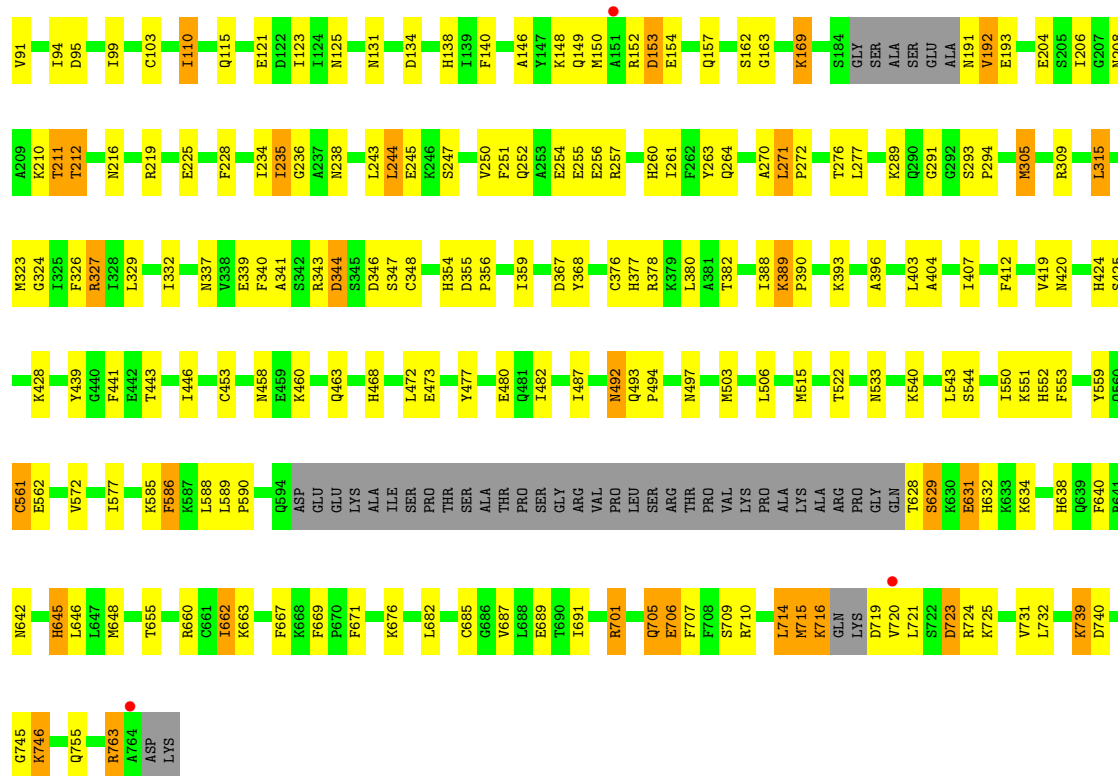
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: MYOSIN VA

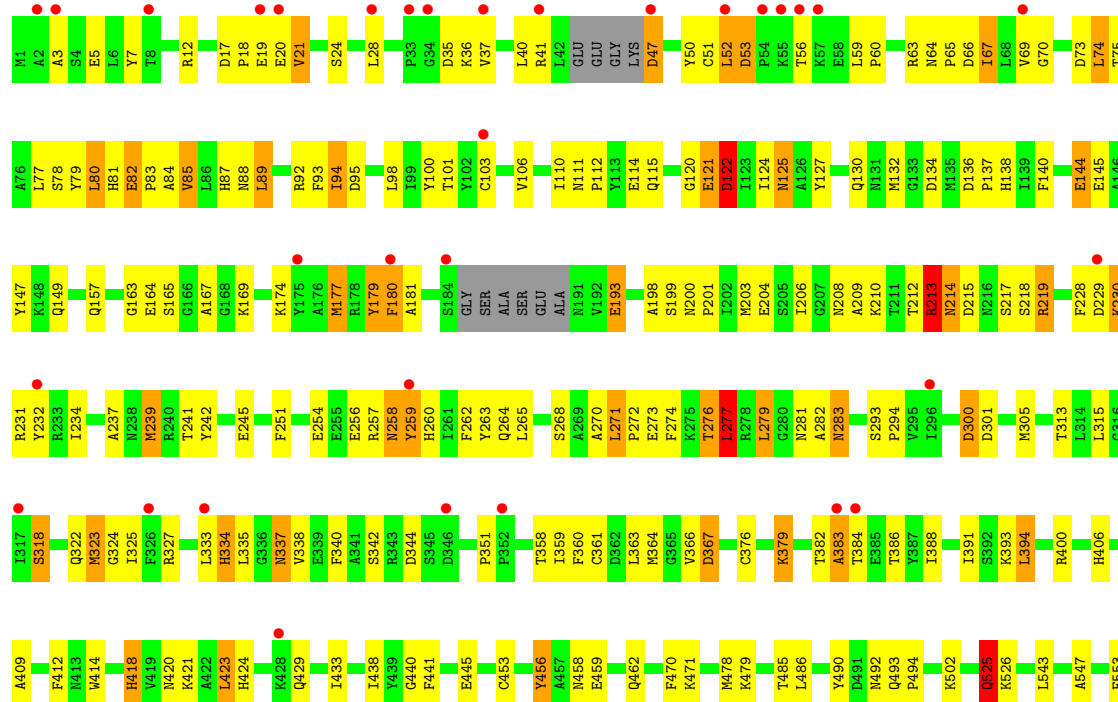


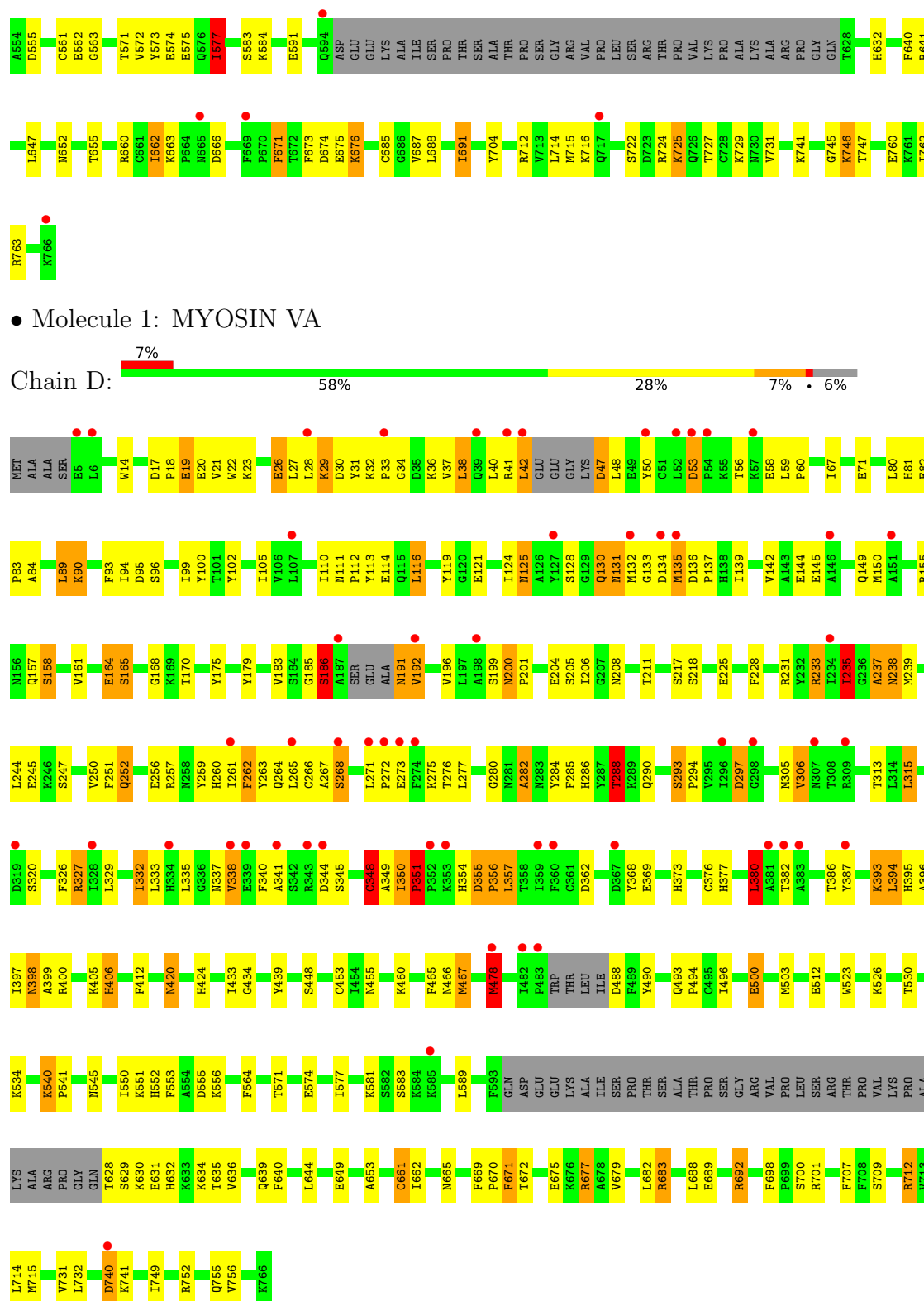
• Molecule 1: MYOSIN VA





• Molecule 1: MYOSIN VA





• Molecule 1: MYOSIN VA

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.48Å 162.31Å 174.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.52 – 2.70 118.91 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (119.52-2.70) 99.9 (118.91-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.62Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.255 , 0.308 0.242 , 0.294	Depositor DCC
R_{free} test set	5924 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22756	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1405e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.12	10/5882 (0.2%)	1.16	11/7963 (0.1%)
1	B	1.06	4/5832 (0.1%)	1.12	10/7901 (0.1%)
1	C	1.06	7/5830 (0.1%)	1.12	12/7897 (0.2%)
1	D	1.06	9/5676 (0.2%)	1.13	7/7701 (0.1%)
All	All	1.08	30/23220 (0.1%)	1.13	40/31462 (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	C	0	1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	478	MET	SD-CE	8.81	2.01	1.79
1	A	503	MET	SD-CE	8.39	2.00	1.79
1	A	478	MET	SD-CE	7.73	1.98	1.79
1	A	469	VAL	CA-CB	7.29	1.62	1.54
1	B	503	MET	SD-CE	7.20	1.97	1.79
1	B	305	MET	SD-CE	-6.91	1.62	1.79
1	C	577	ILE	CA-CB	6.74	1.62	1.54
1	B	763	ARG	C-N	-6.69	1.24	1.33
1	A	203	MET	SD-CE	-6.45	1.63	1.79
1	C	276	THR	CA-CB	6.44	1.61	1.52
1	C	323	MET	SD-CE	6.40	1.95	1.79
1	D	467	MET	SD-CE	6.29	1.95	1.79
1	C	386	THR	CA-C	6.13	1.59	1.52
1	D	386	THR	CA-C	6.13	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	288	THR	CA-CB	6.08	1.61	1.53
1	A	384	THR	CA-CB	6.05	1.63	1.53
1	D	235	ILE	CA-CB	5.97	1.61	1.54
1	C	478	MET	SD-CE	5.91	1.94	1.79
1	C	239	MET	SD-CE	-5.79	1.65	1.79
1	A	515	MET	SD-CE	5.73	1.93	1.79
1	B	99	ILE	C-O	-5.55	1.18	1.24
1	A	105	ILE	C-O	-5.46	1.18	1.24
1	A	73	ASP	C-O	-5.41	1.18	1.24
1	D	500	GLU	N-CA	5.41	1.52	1.45
1	C	41	ARG	NE-CZ	5.26	1.38	1.33
1	A	572	VAL	CA-CB	5.23	1.61	1.54
1	A	41	ARG	CA-C	5.05	1.59	1.52
1	D	478	MET	CG-SD	5.05	1.93	1.80
1	D	545	ASN	CB-CG	-5.04	1.39	1.52
1	D	150	MET	SD-CE	-5.01	1.67	1.79

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	HIS	N-CA-CB	-7.34	98.08	110.49
1	C	409	ALA	N-CA-C	-7.18	103.45	111.28
1	C	386	THR	N-CA-C	7.13	120.04	108.34
1	C	74	LEU	N-CA-C	-7.11	104.47	113.01
1	D	196	VAL	CB-CA-C	-7.11	102.70	112.02
1	A	487	ILE	N-CA-C	6.50	117.71	108.93
1	A	441	PHE	N-CA-C	6.30	119.17	110.35
1	B	250	VAL	CB-CA-C	-6.27	104.50	110.70
1	B	645	HIS	N-CA-C	-6.24	104.40	111.14
1	D	262	PHE	N-CA-C	6.19	117.72	110.97
1	A	640	PHE	N-CA-C	-6.17	104.64	111.36
1	D	380	LEU	N-CA-C	-5.99	100.43	109.95
1	D	630	LYS	N-CA-C	-5.92	103.80	111.02
1	C	149	GLN	N-CA-C	5.84	118.43	111.71
1	A	400	ARG	N-CA-C	-5.76	104.69	110.97
1	A	41	ARG	N-CA-C	5.75	119.06	112.57
1	C	563	GLY	N-CA-C	5.66	121.81	115.08
1	C	213	ARG	N-CA-C	5.65	117.22	110.44
1	A	397	ILE	CB-CA-C	-5.62	104.78	111.97
1	C	525	GLN	N-CA-C	-5.58	105.28	111.36
1	D	500	GLU	N-CA-C	5.52	121.43	114.31
1	B	192	VAL	N-CA-C	5.47	115.60	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	VAL	N-CA-C	5.46	116.09	110.36
1	C	655	THR	N-CA-C	-5.42	102.94	109.72
1	A	412	PHE	N-CA-C	-5.42	105.03	111.69
1	B	561	CYS	N-CA-C	5.41	118.67	111.75
1	D	636	VAL	CB-CA-C	-5.36	104.91	112.14
1	C	456	TYR	N-CA-C	-5.34	105.38	111.14
1	B	70	GLY	N-CA-C	-5.32	104.83	114.46
1	D	327	ARG	N-CA-C	-5.24	105.48	111.14
1	A	6	LEU	N-CA-C	-5.21	107.05	113.41
1	C	547	ALA	N-CA-C	5.17	116.70	108.79
1	B	631	GLU	N-CA-C	5.13	117.27	111.11
1	B	162	SER	N-CA-C	5.11	117.63	109.81
1	B	234	ILE	N-CA-C	5.10	115.62	108.89
1	A	267	ALA	N-CA-C	-5.09	106.76	113.17
1	A	234	ILE	CB-CA-C	-5.08	104.54	111.15
1	C	671	PHE	N-CA-C	5.07	121.61	110.80
1	B	260	HIS	N-CA-C	5.07	117.20	111.11
1	B	235	ILE	N-CA-C	5.01	116.33	112.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	333	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5751	0	5571	132	0
1	B	5701	0	5475	117	0
1	C	5700	0	5469	155	0
1	D	5549	0	5148	146	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	D	5	0	0	1	0
3	A	18	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	13	0	0	1	0
3	D	4	0	0	0	0
All	All	22756	0	21663	550	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 12.

All (550) 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:D:478:MET:CE	1:D:478:MET:SD	2.01	1.48
1:C:110:ILE:HG13	1:C:662:ILE:HD11	1.35	1.09
1:C:103:CYS:SG	1:C:691:ILE:HD11	1.99	1.02
1:C:121:GLU:O	1:C:125:ASN:ND2	2.01	0.92
1:D:204:GLU:HG3	1:D:208:ASN:HD22	1.39	0.88
1:A:41:ARG:H	1:A:41:ARG:NH1	1.73	0.86
1:C:674:ASP:OD2	1:C:676:LYS:HG2	1.76	0.86
1:C:180:PHE:HB3	1:C:234:ILE:HD11	1.59	0.81
1:D:394:LEU:O	1:D:396:ALA:N	2.15	0.80
1:C:81:HIS:NE2	1:C:84:ALA:HB2	1.97	0.79
1:A:144:GLU:OE1	1:A:179:TYR:OH	1.99	0.79
1:D:286:HIS:O	1:D:290:GLN:NE2	2.15	0.79
1:C:18:PRO:O	1:C:676:LYS:NZ	2.17	0.78
1:A:286:HIS:H	1:A:337:ASN:HD21	1.32	0.76
1:C:334:HIS:HE1	1:C:359:ILE:HB	1.51	0.76
1:C:85:VAL:O	1:C:89:LEU:HB2	1.86	0.76
1:A:203:MET:HE3	1:A:239:MET:HE1	1.69	0.74
1:B:84:ALA:O	1:B:88:ASN:ND2	2.20	0.73
1:A:508:LEU:HD12	1:A:527:LEU:HD23	1.71	0.73
1:C:203:MET:SD	1:C:239:MET:HE1	2.29	0.72
1:D:741:LYS:HA	1:D:752:ARG:HG2	1.70	0.72
1:A:733:GLU:HG2	1:A:739:LYS:NZ	2.05	0.72
1:B:354:HIS:ND1	1:B:356:PRO:HD2	2.05	0.72
1:D:465:PHE:HD2	1:D:466:ASN:HD22	1.37	0.71
1:A:464:GLN:HG2	1:A:648:MET:HE1	1.73	0.71
1:D:204:GLU:HG3	1:D:208:ASN:ND2	2.06	0.70
1:A:70:GLY:H	1:A:88:ASN:HD21	1.38	0.70
1:C:382:THR:O	1:C:382:THR:HG23	1.92	0.70
1:B:110:ILE:HD13	1:B:662:ILE:HD11	1.74	0.69
1:D:208:ASN:OD1	1:D:218:SER:HA	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:LYS:O	1:A:586:PHE:HB2	1.92	0.68
1:B:477:TYR:CE1	1:B:487:ILE:HD11	2.29	0.68
1:B:339:GLU:HB3	1:B:354:HIS:HE2	1.59	0.68
1:A:27:LEU:HD11	1:A:38:LEU:HD23	1.76	0.68
1:C:382:THR:O	1:C:384:THR:N	2.27	0.68
1:A:70:GLY:H	1:A:88:ASN:ND2	1.91	0.68
1:A:208:ASN:HD22	1:A:216:ASN:HD21	1.42	0.67
1:C:138:HIS:NE2	1:C:140:PHE:CD2	2.63	0.66
1:A:41:ARG:NH1	1:A:41:ARG:N	2.43	0.66
1:B:705:GLN:NE2	1:B:709:SER:OG	2.29	0.66
1:C:376:CYS:HA	1:C:391:ILE:HD11	1.77	0.66
1:D:628:THR:HG23	1:D:629:SER:H	1.61	0.66
1:A:208:ASN:HD22	1:A:216:ASN:ND2	1.93	0.65
1:D:335:LEU:O	1:D:400:ARG:HD2	1.96	0.65
1:A:281:ASN:C	1:A:281:ASN:HD22	2.03	0.65
1:A:246:LYS:NZ	1:A:639:GLN:HE22	1.95	0.65
1:C:64:ASN:HD21	1:C:79:TYR:N	1.95	0.65
1:B:192:VAL:HG22	1:B:236:GLY:HA2	1.79	0.64
1:A:32:LYS:O	1:A:35:ASP:HB2	1.98	0.64
1:C:74:LEU:HD12	1:C:103:CYS:HB2	1.80	0.64
1:C:264:GLN:HA	1:C:301:ASP:HB3	1.79	0.64
1:B:629:SER:HA	1:B:632:HIS:ND1	2.13	0.64
1:D:677:ARG:O	1:D:677:ARG:HG3	1.97	0.64
1:A:733:GLU:HG2	1:A:739:LYS:HZ3	1.62	0.64
1:D:145:GLU:OE1	1:D:149:GLN:NE2	2.30	0.64
1:D:239:MET:H	1:D:420:ASN:HD21	1.46	0.64
1:A:41:ARG:H	1:A:41:ARG:CZ	2.11	0.63
1:B:634:LYS:HZ2	1:B:642:ASN:HD21	1.45	0.63
1:C:77:LEU:HD21	1:C:88:ASN:HD22	1.63	0.63
1:A:41:ARG:N	1:A:41:ARG:CZ	2.62	0.63
1:A:463:GLN:NE2	1:A:491:ASP:OD1	2.30	0.62
1:D:29:LYS:HG2	1:D:30:ASP:H	1.64	0.62
1:B:153:ASP:O	1:B:154:GLU:C	2.41	0.62
1:C:334:HIS:HE1	1:C:359:ILE:CB	2.13	0.62
1:B:403:LEU:O	1:B:407:ILE:HG13	2.00	0.62
1:D:59:LEU:HD12	1:D:59:LEU:H	1.64	0.62
1:B:634:LYS:HD3	1:B:638:HIS:ND1	2.14	0.62
1:C:360:PHE:O	1:C:364:MET:HG2	2.00	0.62
1:D:257:ARG:HG2	1:D:263:TYR:CE2	2.35	0.61
1:D:266:CYS:HB3	1:D:280:GLY:O	2.00	0.61
1:C:414:TRP:CZ2	1:C:418:HIS:CD2	2.89	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ARG:HG2	1:D:263:TYR:CZ	2.35	0.60
1:D:665:ASN:HD21	1:D:669:PHE:H	1.47	0.60
1:D:355:ASP:HB2	1:D:356:PRO:HD3	1.81	0.60
1:C:228:PHE:CE1	1:C:234:ILE:HD13	2.36	0.60
1:C:281:ASN:O	1:C:283:ASN:N	2.34	0.60
1:D:373:HIS:NE2	1:D:377:HIS:HD2	1.98	0.60
1:C:283:ASN:N	1:C:283:ASN:OD1	2.33	0.60
1:D:268:SER:OG	1:D:305:MET:HG3	2.02	0.59
1:A:468:HIS:CE1	1:A:656:PRO:HD2	2.38	0.59
1:C:525:GLN:HG3	3:C:2008:HOH:O	2.03	0.59
1:C:204:GLU:O	1:C:208:ASN:HB2	2.03	0.59
1:A:7:TYR:CZ	1:A:62:LEU:HD12	2.38	0.58
1:C:64:ASN:HD21	1:C:79:TYR:H	1.50	0.58
1:C:340:PHE:O	1:C:393:LYS:HE3	2.03	0.58
1:D:465:PHE:HD2	1:D:466:ASN:ND2	2.00	0.58
1:A:41:ARG:NH2	1:A:42:LEU:N	2.51	0.58
1:B:3:ALA:C	1:B:5:GLU:H	2.12	0.58
1:A:2:ALA:O	1:A:4:SER:N	2.36	0.58
1:D:225:GLU:O	1:D:237:ALA:HA	2.03	0.58
1:D:157:GLN:O	1:D:433:ILE:HA	2.03	0.57
1:D:102:TYR:CD1	1:D:137:PRO:HB3	2.39	0.57
1:C:660:ARG:HD2	1:C:685:CYS:HB3	1.85	0.57
1:B:121:GLU:O	1:B:125:ASN:ND2	2.37	0.56
1:C:198:ALA:O	1:C:201:PRO:HD2	2.04	0.56
1:B:81:HIS:HD1	1:B:83:PRO:HG2	1.69	0.56
1:A:712:ARG:O	1:A:715:MET:HG2	2.06	0.56
1:C:100:TYR:HB2	1:C:137:PRO:O	2.06	0.56
1:D:125:ASN:H	1:D:125:ASN:HD22	1.54	0.56
1:D:164:GLU:O	1:D:165:SER:C	2.49	0.56
1:D:341:ALA:O	1:D:348:CYS:HA	2.05	0.56
1:D:155:ARG:NH2	1:D:653:ALA:O	2.39	0.56
1:A:368:TYR:C	1:A:368:TYR:CD2	2.84	0.56
1:C:459:GLU:OE2	1:C:553:PHE:N	2.39	0.56
1:D:29:LYS:H	1:D:29:LYS:HD3	1.70	0.56
1:A:464:GLN:NE2	1:A:658:TYR:OH	2.39	0.56
1:D:329:LEU:O	1:D:333:LEU:HG	2.05	0.55
1:C:100:TYR:CD2	1:C:138:HIS:HA	2.41	0.55
1:C:77:LEU:HD21	1:C:88:ASN:ND2	2.21	0.55
1:D:373:HIS:NE2	1:D:377:HIS:CD2	2.73	0.55
1:C:242:TYR:CD2	1:C:647:LEU:HD13	2.41	0.55
1:C:24:SER:OG	1:C:63:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:THR:O	1:C:382:THR:CG2	2.54	0.55
1:C:727:THR:O	1:C:731:VAL:HG23	2.07	0.55
1:A:85:VAL:HG21	1:A:691:ILE:HD13	1.89	0.55
1:A:229:ASP:OD1	1:A:231:ARG:N	2.40	0.54
1:A:110:ILE:HD12	1:A:110:ILE:N	2.22	0.54
1:C:414:TRP:CH2	1:C:418:HIS:CD2	2.96	0.54
1:C:490:TYR:HE2	1:C:492:ASN:HB3	1.73	0.54
1:D:144:GLU:OE1	1:D:179:TYR:OH	2.22	0.54
1:A:719:ASP:O	1:A:721:LEU:HD12	2.08	0.54
1:C:7:TYR:CD1	1:C:59:LEU:HD13	2.42	0.54
1:D:493:GLN:N	1:D:494:PRO:CD	2.70	0.54
1:A:9:LYS:CB	1:A:30:ASP:OD1	2.56	0.54
1:A:105:ILE:C	1:A:105:ILE:HD12	2.33	0.54
1:B:389:LYS:HG2	1:B:390:PRO:O	2.08	0.54
1:A:708:PHE:CE2	1:A:712:ARG:HG2	2.43	0.53
1:C:136:ASP:HB3	1:C:137:PRO:HD2	1.90	0.53
1:C:144:GLU:HG2	1:C:179:TYR:OH	2.07	0.53
1:A:41:ARG:C	1:A:41:ARG:NE	2.67	0.53
1:B:163:GLY:O	1:B:169:LYS:HE3	2.09	0.53
1:D:37:VAL:HA	1:D:50:TYR:O	2.08	0.53
1:B:71:GLU:OE1	1:B:71:GLU:HA	2.09	0.53
1:D:17:ASP:OD2	1:D:19:GLU:OE1	2.26	0.53
1:D:37:VAL:C	1:D:38:LEU:HD23	2.34	0.53
1:D:204:GLU:O	1:D:208:ASN:HB2	2.09	0.53
1:D:631:GLU:HA	1:D:634:LYS:HG3	1.91	0.53
1:C:391:ILE:HD12	1:C:391:ILE:O	2.09	0.53
1:D:111:ASN:OD1	1:D:112:PRO:HD2	2.09	0.52
1:A:443:THR:HG22	1:A:447:ASN:HD21	1.75	0.52
1:C:81:HIS:ND1	1:C:83:PRO:HD2	2.24	0.52
1:C:335:LEU:O	1:C:400:ARG:HD2	2.08	0.52
1:B:305:MET:HE1	1:B:326:PHE:CE1	2.44	0.52
1:D:263:TYR:OH	1:D:288:THR:HA	2.09	0.52
1:A:82:GLU:HB3	1:A:83:PRO:HD3	1.91	0.52
1:D:208:ASN:HA	1:D:217:SER:O	2.08	0.52
1:A:698:PHE:CE1	1:A:743:GLN:NE2	2.77	0.52
1:C:257:ARG:C	1:C:258:ASN:O	2.45	0.52
1:C:87:HIS:O	1:C:88:ASN:C	2.53	0.52
1:A:430:HIS:C	1:A:430:HIS:HD1	2.18	0.52
1:B:41:ARG:HG3	1:B:41:ARG:HH11	1.75	0.52
1:D:455:ASN:HB3	1:D:552:HIS:CD2	2.45	0.52
1:D:251:PHE:C	1:D:252:GLN:HE21	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LEU:HD21	1:B:41:ARG:HB2	1.92	0.51
1:B:344:ASP:OD1	1:B:347:SER:HB3	2.10	0.51
1:B:714:LEU:HD21	1:B:763:ARG:HG3	1.91	0.51
1:A:327:ARG:HD3	1:A:586:PHE:CE1	2.45	0.51
1:B:480:GLU:HA	1:B:480:GLU:OE2	2.11	0.51
1:C:691:ILE:N	1:C:691:ILE:HD13	2.25	0.51
1:D:397:ILE:C	1:D:399:ALA:H	2.19	0.51
1:D:698:PHE:CE2	1:D:752:ARG:HD3	2.45	0.51
1:A:41:ARG:O	1:A:42:LEU:C	2.53	0.51
1:B:468:HIS:CE1	1:B:472:LEU:HD11	2.45	0.51
1:B:103:CYS:SG	1:B:691:ILE:HD11	2.51	0.51
1:A:512:GLU:HG2	1:A:523:TRP:HB2	1.93	0.51
1:C:138:HIS:CD2	1:C:140:PHE:H	2.29	0.51
1:A:36:LYS:HD2	1:A:36:LYS:N	2.25	0.51
1:C:704:TYR:CD2	1:C:725:LYS:HG3	2.46	0.51
1:A:315:LEU:HD22	1:A:419:VAL:HG13	1.93	0.50
1:C:163:GLY:O	1:C:169:LYS:HE3	2.12	0.50
1:C:406:HIS:CD2	1:C:577:ILE:HD11	2.46	0.50
1:D:124:ILE:HG23	1:D:179:TYR:CD1	2.46	0.50
1:D:677:ARG:O	1:D:677:ARG:CG	2.59	0.50
1:A:184:SER:HB2	1:A:233:ARG:HA	1.92	0.50
1:B:138:HIS:HD2	1:B:140:PHE:CG	2.29	0.50
1:B:705:GLN:O	1:B:706:GLU:C	2.53	0.50
1:B:3:ALA:C	1:B:5:GLU:N	2.69	0.50
1:B:715:MET:HG2	1:B:731:VAL:HG11	1.93	0.50
1:C:270:ALA:O	1:C:271:LEU:HD23	2.11	0.50
1:D:628:THR:HG23	1:D:629:SER:N	2.26	0.50
1:C:40:LEU:HD12	1:C:50:TYR:HB2	1.94	0.50
1:C:179:TYR:O	1:C:180:PHE:C	2.54	0.50
1:A:229:ASP:OD1	1:A:229:ASP:C	2.54	0.50
1:B:550:ILE:N	1:B:550:ILE:HD12	2.27	0.50
1:B:720:VAL:O	1:B:720:VAL:HG23	2.12	0.50
1:D:121:GLU:HA	1:D:124:ILE:HD12	1.94	0.50
1:B:270:ALA:O	1:B:271:LEU:C	2.54	0.50
1:C:300:ASP:OD2	1:C:300:ASP:C	2.54	0.50
1:D:337:ASN:O	1:D:338:VAL:C	2.54	0.50
1:B:251:PHE:CD2	1:B:252:GLN:N	2.80	0.50
1:B:441:PHE:CE2	1:B:458:ASN:HB3	2.47	0.50
1:B:710:ARG:O	1:B:763:ARG:NE	2.43	0.50
1:B:477:TYR:CD1	1:B:487:ILE:HD11	2.46	0.50
1:B:716:LYS:O	1:B:719:ASP:OD1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:VAL:HG12	1:C:51:CYS:HA	1.93	0.50
1:C:180:PHE:CB	1:C:234:ILE:HD11	2.36	0.50
1:D:191:ASN:HD22	1:D:192:VAL:H	1.59	0.50
1:C:462:GLN:NE2	1:C:553:PHE:CE2	2.80	0.50
1:B:152:ARG:C	1:B:153:ASP:OD1	2.55	0.49
1:C:277:LEU:HD23	1:C:279:LEU:HD21	1.93	0.49
1:A:52:LEU:HD23	1:A:52:LEU:H	1.76	0.49
1:C:147:TYR:OH	1:C:232:TYR:O	2.24	0.49
1:C:177:MET:HE2	1:C:193:GLU:HA	1.95	0.49
1:B:251:PHE:CD2	1:B:251:PHE:C	2.90	0.49
1:C:414:TRP:CH2	1:C:418:HIS:HD2	2.30	0.49
1:A:705:GLN:O	1:A:706:GLU:C	2.55	0.49
1:C:334:HIS:CE1	1:C:359:ILE:HB	2.38	0.49
1:D:28:LEU:HD21	1:D:41:ARG:HB2	1.95	0.49
1:A:675:GLU:O	1:A:679:VAL:HG23	2.12	0.49
1:B:420:ASN:O	1:B:424:HIS:ND1	2.45	0.49
1:B:586:PHE:N	1:B:586:PHE:CD2	2.81	0.49
1:C:334:HIS:HE1	1:C:359:ILE:CG2	2.25	0.49
1:D:238:ASN:OD1	1:D:424:HIS:HE1	1.95	0.49
1:A:110:ILE:HD13	3:A:2004:HOH:O	2.12	0.49
1:A:364:MET:N	1:A:364:MET:HE2	2.26	0.49
1:A:430:HIS:O	1:A:430:HIS:ND1	2.39	0.49
1:B:315:LEU:HD22	1:B:419:VAL:HG13	1.95	0.49
1:C:277:LEU:HA	1:C:363:LEU:HD21	1.95	0.49
1:D:119:TYR:CD2	1:D:175:TYR:CE2	3.00	0.49
1:D:369:GLU:OE1	1:D:369:GLU:HA	2.13	0.49
1:D:679:VAL:HG12	1:D:683:ARG:NH2	2.28	0.49
1:C:265:LEU:HA	1:C:305:MET:HE3	1.95	0.49
1:D:27:LEU:HD23	1:D:40:LEU:HD23	1.94	0.49
1:A:254:GLU:O	1:A:255:GLU:HB2	2.12	0.49
1:A:588:LEU:O	1:A:591:GLU:HB2	2.13	0.49
1:A:670:PRO:O	1:A:671:PHE:C	2.56	0.49
1:D:629:SER:HA	1:D:632:HIS:ND1	2.28	0.48
1:C:103:CYS:N	1:C:106:VAL:O	2.42	0.48
1:B:460:LYS:NZ	1:B:645:HIS:NE2	2.62	0.48
1:C:662:ILE:H	1:C:662:ILE:HD13	1.78	0.48
1:D:380:LEU:N	1:D:380:LEU:CD2	2.76	0.48
1:A:330:ALA:HA	1:A:333:LEU:HD12	1.95	0.48
1:C:213:ARG:O	1:C:214:ASN:HB2	2.12	0.48
1:D:490:TYR:C	1:D:490:TYR:CD2	2.91	0.48
1:B:225:GLU:HG3	1:B:238:ASN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:LYS:HD2	1:C:575:GLU:OE2	2.14	0.48
1:A:552:HIS:HB2	1:A:555:ASP:O	2.14	0.48
1:B:41:ARG:HH12	1:B:47:ASP:HA	1.78	0.48
1:D:27:LEU:HD23	1:D:40:LEU:CD2	2.44	0.48
1:A:405:LYS:HE3	1:A:570:ASP:OD1	2.13	0.48
1:C:485:THR:HG22	1:C:485:THR:O	2.14	0.48
1:B:367:ASP:O	1:B:368:TYR:C	2.54	0.48
1:D:211:THR:HA	1:D:256:GLU:HG2	1.96	0.48
1:A:354:HIS:CD2	1:A:356:PRO:HD2	2.49	0.48
1:B:332:ILE:HG23	1:B:404:ALA:HB1	1.96	0.48
1:C:412:PHE:C	1:C:412:PHE:CD2	2.92	0.48
1:C:453:CYS:HB3	1:C:640:PHE:CZ	2.49	0.48
1:A:246:LYS:NZ	1:A:570:ASP:OD2	2.46	0.48
1:C:17:ASP:O	1:C:21:VAL:HA	2.13	0.48
1:C:110:ILE:HD12	1:C:110:ILE:N	2.28	0.48
1:D:206:ILE:HD12	1:D:412:PHE:CD1	2.49	0.48
1:A:450:GLU:OE2	1:A:567:LYS:NZ	2.47	0.47
1:A:496:ILE:O	1:A:500:GLU:HG2	2.13	0.47
1:A:568:ASN:O	1:A:635:THR:HB	2.14	0.47
1:C:179:TYR:O	1:C:181:ALA:N	2.47	0.47
1:D:332:ILE:N	1:D:332:ILE:HD13	2.29	0.47
1:D:406:HIS:HD2	1:D:577:ILE:HD11	1.79	0.47
1:A:720:VAL:HG12	1:A:720:VAL:O	2.12	0.47
1:B:420:ASN:HB3	1:B:424:HIS:CE1	2.49	0.47
1:D:265:LEU:HD13	1:D:326:PHE:CD1	2.49	0.47
1:A:367:ASP:O	1:A:368:TYR:C	2.54	0.47
1:D:29:LYS:CG	1:D:30:ASP:N	2.75	0.47
1:D:670:PRO:O	1:D:671:PHE:C	2.56	0.47
1:B:355:ASP:O	1:B:359:ILE:HG12	2.14	0.47
1:A:9:LYS:O	1:A:10:TYR:CB	2.62	0.47
1:A:468:HIS:HE1	1:A:656:PRO:HD2	1.79	0.47
1:B:270:ALA:O	1:B:271:LEU:O	2.32	0.47
1:C:462:GLN:HG2	1:C:553:PHE:CD2	2.49	0.47
1:D:252:GLN:NE2	1:D:252:GLN:N	2.62	0.47
1:D:280:GLY:HA3	1:D:284:TYR:HD2	1.78	0.47
1:B:553:PHE:CZ	1:B:689:GLU:HB3	2.48	0.47
1:A:70:GLY:N	1:A:88:ASN:HD21	2.10	0.47
1:A:246:LYS:HZ1	1:A:639:GLN:HE22	1.62	0.47
1:A:443:THR:HG23	1:A:557:VAL:HG13	1.97	0.47
1:B:271:LEU:O	1:B:272:PRO:C	2.57	0.47
1:C:81:HIS:CE1	1:C:84:ALA:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ASN:H	1:D:125:ASN:ND2	2.11	0.47
1:D:228:PHE:HD1	1:D:233:ARG:C	2.22	0.47
1:D:741:LYS:HD2	1:D:755:GLN:NE2	2.30	0.47
1:A:439:TYR:CE2	1:A:454:ILE:HG23	2.49	0.47
1:D:29:LYS:HG2	1:D:30:ASP:N	2.30	0.47
1:C:318:SER:O	1:C:322:GLN:HB2	2.15	0.47
1:A:439:TYR:CD2	1:A:454:ILE:HG23	2.50	0.47
1:D:185:GLY:O	1:D:186:SER:O	2.32	0.47
1:D:682:LEU:HB3	1:D:688:LEU:HD13	1.97	0.47
1:B:293:SER:O	1:B:294:PRO:C	2.56	0.46
1:B:687:VAL:O	1:B:691:ILE:HG12	2.15	0.46
1:D:14:TRP:O	1:D:60:PRO:HB2	2.15	0.46
1:D:707:PHE:CZ	1:D:732:LEU:HD13	2.50	0.46
1:A:589:LEU:N	1:A:590:PRO:HD2	2.30	0.46
1:A:733:GLU:HG2	1:A:739:LYS:HZ2	1.78	0.46
1:B:146:ALA:O	1:B:157:GLN:HG3	2.15	0.46
1:D:280:GLY:HA3	1:D:284:TYR:CD2	2.50	0.46
1:B:254:GLU:O	1:B:255:GLU:HB2	2.15	0.46
1:C:53:ASP:OD1	1:C:53:ASP:N	2.47	0.46
1:C:181:ALA:HA	1:C:234:ILE:HG12	1.98	0.46
1:C:361:CYS:HB3	1:C:366:VAL:O	2.15	0.46
1:D:260:HIS:O	1:D:261:ILE:C	2.59	0.46
1:C:47:ASP:OD1	1:C:47:ASP:N	2.47	0.46
1:C:81:HIS:CD2	1:C:84:ALA:HB2	2.50	0.46
1:C:258:ASN:HD22	1:C:262:PHE:HD2	1.63	0.46
1:C:572:VAL:HG12	1:C:632:HIS:HB3	1.98	0.46
1:A:335:LEU:HD21	1:A:403:LEU:HD23	1.96	0.46
1:B:589:LEU:HB3	1:B:590:PRO:HD3	1.98	0.46
1:A:670:PRO:O	1:A:672:THR:OG1	2.30	0.46
1:C:379:LYS:HE2	1:C:388:ILE:HD11	1.98	0.46
1:A:264:GLN:HB3	1:A:305:MET:HB2	1.97	0.46
1:C:7:TYR:OH	1:C:60:PRO:O	2.31	0.46
1:D:540:LYS:NZ	1:D:541:PRO:O	2.48	0.46
1:A:530:THR:HG22	1:A:531:HIS:CE1	2.51	0.46
1:B:41:ARG:HH12	1:B:47:ASP:CA	2.29	0.46
1:B:324:GLY:C	1:B:588:LEU:HD23	2.40	0.46
1:B:745:GLY:O	1:B:746:LYS:C	2.59	0.46
1:A:206:ILE:HD12	1:A:412:PHE:CD1	2.51	0.46
1:D:47:ASP:O	1:D:48:LEU:HG	2.16	0.46
1:A:200:ASN:O	1:A:204:GLU:HG3	2.16	0.45
1:B:341:ALA:O	1:B:348:CYS:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:LEU:CD2	1:D:110:ILE:HD11	2.46	0.45
1:A:77:LEU:O	1:A:80:LEU:HD21	2.15	0.45
1:C:334:HIS:CE1	1:C:359:ILE:CG2	2.99	0.45
1:C:493:GLN:N	1:C:494:PRO:CD	2.78	0.45
1:D:496:ILE:O	1:D:500:GLU:HG2	2.16	0.45
1:D:740:ASP:C	1:D:740:ASP:OD1	2.59	0.45
1:A:364:MET:HE2	1:A:364:MET:CA	2.46	0.45
1:C:394:LEU:HD12	1:C:394:LEU:O	2.16	0.45
1:A:249:VAL:HG12	1:A:249:VAL:O	2.16	0.45
1:C:673:PHE:HE2	1:C:675:GLU:HG3	1.82	0.45
1:D:168:GLY:HA2	2:D:1767:SO4:O3	2.16	0.45
1:D:368:TYR:O	1:D:368:TYR:CD1	2.70	0.45
1:B:453:CYS:HB3	1:B:640:PHE:CZ	2.51	0.45
1:D:42:LEU:HD21	1:D:48:LEU:HD11	1.97	0.45
1:D:199:SER:HB3	1:D:315:LEU:HD11	1.98	0.45
1:D:200:ASN:N	1:D:201:PRO:CD	2.79	0.45
1:A:453:CYS:HB3	1:A:640:PHE:CE1	2.52	0.45
1:B:482:ILE:HD11	1:B:745:GLY:CA	2.46	0.45
1:B:739:LYS:CD	1:B:739:LYS:H	2.30	0.45
1:C:167:ALA:HB2	1:C:663:LYS:HB2	1.99	0.45
1:C:367:ASP:OD2	1:C:367:ASP:N	2.27	0.45
1:B:131:ASN:HB2	1:B:134:ASP:OD2	2.16	0.45
1:B:257:ARG:HB3	1:B:263:TYR:CE2	2.52	0.45
1:D:350:ILE:O	1:D:351:PRO:C	2.59	0.45
1:A:296:ILE:HB	1:A:299:ILE:CG2	2.47	0.45
1:D:453:CYS:HB3	1:D:640:PHE:CZ	2.51	0.45
1:A:463:GLN:HA	1:A:463:GLN:OE1	2.16	0.45
1:B:561:CYS:O	1:B:562:GLU:C	2.60	0.45
1:C:80:LEU:HG	1:C:691:ILE:HG23	1.99	0.45
1:A:698:PHE:HB3	1:A:750:PHE:HB3	1.99	0.45
1:B:211:THR:OG1	1:B:212:THR:N	2.49	0.45
1:C:440:GLY:O	1:C:441:PHE:C	2.60	0.45
1:B:206:ILE:HD12	1:B:412:PHE:CD1	2.52	0.44
1:B:81:HIS:ND1	1:B:83:PRO:HG2	2.32	0.44
1:C:745:GLY:O	1:C:746:LYS:C	2.60	0.44
1:D:56:THR:HG22	1:D:58:GLU:HB2	1.98	0.44
1:B:453:CYS:HB3	1:B:640:PHE:CE1	2.52	0.44
1:C:324:GLY:O	1:C:325:ILE:C	2.58	0.44
1:D:340:PHE:HB2	1:D:393:LYS:HD3	1.99	0.44
1:A:364:MET:O	1:A:583:SER:OG	2.22	0.44
1:C:28:LEU:HD12	1:C:40:LEU:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ASN:ND2	1:C:262:PHE:CD2	2.84	0.44
1:D:523:TRP:CH2	1:D:564:PHE:CD1	3.06	0.44
1:A:325:ILE:HD11	1:A:414:TRP:CZ3	2.52	0.44
1:B:138:HIS:CD2	1:B:140:PHE:H	2.36	0.44
1:A:350:ILE:HD12	1:A:376:CYS:SG	2.57	0.44
1:B:138:HIS:HD2	1:B:140:PHE:CB	2.31	0.44
1:B:150:MET:HE1	1:B:228:PHE:CD2	2.52	0.44
1:D:81:HIS:CE1	1:D:84:ALA:H	2.36	0.44
1:D:466:ASN:HD22	1:D:466:ASN:N	2.14	0.44
1:A:22:TRP:CD2	1:A:83:PRO:HG3	2.53	0.44
1:A:703:THR:OG1	1:A:706:GLU:HG3	2.18	0.44
1:B:9:LYS:O	1:B:10:TYR:HB2	2.18	0.44
1:B:157:GLN:NE2	1:B:655:THR:HB	2.32	0.44
1:C:111:ASN:OD1	1:C:112:PRO:HD2	2.18	0.44
1:A:453:CYS:HB3	1:A:640:PHE:CZ	2.53	0.44
1:B:38:LEU:HB3	1:B:40:LEU:HD21	1.98	0.44
1:C:337:ASN:O	1:C:338:VAL:C	2.61	0.44
1:D:81:HIS:ND1	1:D:83:PRO:HD2	2.33	0.44
1:D:293:SER:N	1:D:294:PRO:CD	2.81	0.44
1:B:244:LEU:HD22	1:B:245:GLU:H	1.83	0.44
1:D:285:PHE:CE1	1:D:333:LEU:HB3	2.52	0.44
1:A:700:SER:HB2	1:A:751:PHE:HB2	2.00	0.43
1:B:138:HIS:CD2	1:B:140:PHE:CG	3.06	0.43
1:C:237:ALA:HB3	1:C:423:LEU:HG	1.99	0.43
1:C:420:ASN:O	1:C:424:HIS:CD2	2.71	0.43
1:A:64:ASN:N	1:A:64:ASN:HD22	2.15	0.43
1:A:572:VAL:HG12	1:A:632:HIS:HB2	2.01	0.43
1:B:153:ASP:OD1	1:B:153:ASP:N	2.50	0.43
1:B:660:ARG:HD2	1:B:685:CYS:HB3	1.99	0.43
1:C:80:LEU:HG	1:C:691:ILE:CG2	2.48	0.43
1:D:29:LYS:CG	1:D:30:ASP:H	2.25	0.43
1:D:244:LEU:HD12	1:D:245:GLU:H	1.84	0.43
1:B:473:GLU:CD	1:B:701:ARG:HH22	2.25	0.43
1:D:94:ILE:HG22	1:D:95:ASP:OD2	2.17	0.43
1:D:670:PRO:O	1:D:672:THR:N	2.51	0.43
1:A:588:LEU:O	1:A:591:GLU:N	2.51	0.43
1:B:261:ILE:HD13	1:B:329:LEU:HD11	1.99	0.43
1:B:667:PHE:HB2	1:B:669:PHE:CE2	2.53	0.43
1:B:721:LEU:HD12	1:B:721:LEU:N	2.32	0.43
1:C:157:GLN:HB2	1:C:433:ILE:HG23	1.99	0.43
1:D:32:LYS:O	1:D:34:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ASP:OD1	1:D:56:THR:HB	2.19	0.43
1:A:580:LEU:C	1:A:582:SER:H	2.25	0.43
1:A:716:LYS:O	1:A:719:ASP:OD1	2.36	0.43
1:C:93:PHE:HA	1:C:98:LEU:O	2.19	0.43
1:A:430:HIS:C	1:A:430:HIS:ND1	2.77	0.43
1:D:111:ASN:ND2	1:D:113:TYR:CE1	2.86	0.43
1:D:460:LYS:HG3	1:D:644:LEU:HD21	2.00	0.43
1:A:276:THR:HG23	1:A:277:LEU:HD22	2.01	0.43
1:B:243:LEU:O	1:B:244:LEU:C	2.61	0.43
1:C:462:GLN:HG2	1:C:553:PHE:CG	2.54	0.43
1:C:577:ILE:HD12	1:C:577:ILE:HA	1.84	0.43
1:C:712:ARG:HA	1:C:715:MET:HG3	2.00	0.43
1:D:133:GLY:O	1:D:135:MET:N	2.52	0.43
1:D:503:MET:HE2	1:D:503:MET:HA	2.01	0.43
1:A:41:ARG:HH21	1:A:42:LEU:CA	2.31	0.43
1:A:105:ILE:C	1:A:105:ILE:CD1	2.91	0.43
1:A:146:ALA:HB2	1:A:657:HIS:HD2	1.83	0.43
1:B:81:HIS:O	1:B:82:GLU:C	2.62	0.43
1:C:69:VAL:HG12	1:C:70:GLY:N	2.34	0.43
1:D:158:SER:HA	1:D:434:GLY:O	2.19	0.43
1:D:262:PHE:CD1	1:D:333:LEU:HD21	2.54	0.43
1:A:8:THR:OG1	1:A:9:LYS:N	2.52	0.43
1:A:41:ARG:HA	1:A:47:ASP:CG	2.43	0.43
1:A:493:GLN:N	1:A:494:PRO:CD	2.81	0.43
1:B:41:ARG:HH11	1:B:41:ARG:CG	2.30	0.43
1:C:271:LEU:C	1:C:273:GLU:H	2.27	0.43
1:C:490:TYR:CE2	1:C:492:ASN:HB3	2.54	0.43
1:D:21:VAL:HG12	1:D:22:TRP:CD1	2.54	0.43
1:D:90:LYS:O	1:D:93:PHE:N	2.52	0.43
1:D:112:PRO:HG3	1:D:116:LEU:HD12	2.00	0.43
1:A:41:ARG:HH21	1:A:42:LEU:HA	1.84	0.43
1:B:492:ASN:HD22	1:B:492:ASN:H	1.66	0.43
1:B:707:PHE:CZ	1:B:732:LEU:HD13	2.54	0.43
1:B:552:HIS:NE2	1:B:559:TYR:OH	2.41	0.42
1:B:2:ALA:O	1:B:6:LEU:HG	2.19	0.42
1:C:456:TYR:OH	1:C:641:ARG:HG3	2.19	0.42
1:D:264:GLN:O	1:D:267:ALA:HB3	2.18	0.42
1:D:305:MET:O	1:D:306:VAL:C	2.62	0.42
1:A:28:LEU:HD21	1:A:41:ARG:HB3	2.00	0.42
1:A:238:ASN:OD1	1:A:420:ASN:ND2	2.52	0.42
1:B:34:GLY:O	1:B:35:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:ASN:O	1:D:204:GLU:HB2	2.20	0.42
1:B:631:GLU:OE1	1:B:634:LYS:HE3	2.19	0.42
1:C:127:TYR:OH	1:C:136:ASP:O	2.31	0.42
1:B:264:GLN:HB3	1:B:305:MET:HB2	2.02	0.42
1:D:233:ARG:NH1	1:D:235:ILE:HG22	2.34	0.42
1:D:252:GLN:HG2	1:D:257:ARG:HA	2.02	0.42
1:D:675:GLU:O	1:D:679:VAL:HG23	2.19	0.42
1:A:38:LEU:HD22	1:A:40:LEU:HD21	2.02	0.42
1:B:482:ILE:HD11	1:B:745:GLY:HA2	2.02	0.42
1:C:110:ILE:HG13	1:C:662:ILE:CD1	2.25	0.42
1:C:120:GLY:C	1:C:122:ASP:N	2.76	0.42
1:C:209:ALA:HA	1:C:260:HIS:CE1	2.54	0.42
1:D:99:ILE:HG13	1:D:100:TYR:CD1	2.54	0.42
1:A:468:HIS:ND1	1:A:656:PRO:HG2	2.35	0.42
1:B:648:MET:HA	1:B:648:MET:HE3	2.02	0.42
1:D:47:ASP:N	1:D:47:ASP:OD2	2.51	0.42
1:D:553:PHE:CZ	1:D:689:GLU:HG3	2.54	0.42
1:A:40:LEU:HA	1:A:41:ARG:NH1	2.35	0.42
1:A:80:LEU:N	1:A:80:LEU:CD2	2.83	0.42
1:D:130:GLN:C	1:D:131:ASN:ND2	2.78	0.42
1:A:708:PHE:C	1:A:708:PHE:CD2	2.97	0.42
1:B:138:HIS:CD2	1:B:140:PHE:CD2	3.08	0.42
1:B:204:GLU:HG2	1:B:208:ASN:ND2	2.35	0.42
1:B:388:ILE:HD12	1:B:388:ILE:N	2.35	0.42
1:C:64:ASN:ND2	1:C:79:TYR:HB2	2.34	0.42
1:D:340:PHE:CE2	1:D:396:ALA:HB1	2.54	0.42
1:D:420:ASN:O	1:D:424:HIS:CD2	2.73	0.42
1:A:317:ILE:CD1	1:A:418:HIS:HB3	2.50	0.41
1:A:532:LEU:HD13	1:A:540:LYS:HB2	2.01	0.41
1:B:3:ALA:O	1:B:5:GLU:N	2.53	0.41
1:B:256:GLU:O	1:B:291:GLY:HA3	2.20	0.41
1:B:91:VAL:O	1:B:95:ASP:HB2	2.20	0.41
1:B:323:MET:O	1:B:327:ARG:HB2	2.20	0.41
1:C:219:ARG:HG3	1:C:245:GLU:OE2	2.21	0.41
1:C:251:PHE:C	1:C:251:PHE:CD2	2.98	0.41
1:C:561:CYS:O	1:C:562:GLU:C	2.63	0.41
1:C:94:ILE:O	1:C:95:ASP:C	2.63	0.41
1:C:383:ALA:O	1:C:384:THR:C	2.62	0.41
1:C:470:PHE:C	1:C:470:PHE:CD2	2.98	0.41
1:D:82:GLU:HB2	1:D:83:PRO:HD3	2.02	0.41
1:D:282:ALA:HB3	1:D:294:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:550:ILE:CG2	1:D:552:HIS:CE1	3.03	0.41
1:A:473:GLU:HB3	1:A:487:ILE:HD13	2.02	0.41
1:B:493:GLN:N	1:B:494:PRO:CD	2.83	0.41
1:C:92:ARG:NE	1:C:101:THR:HG23	2.35	0.41
1:C:212:THR:OG1	1:C:213:ARG:HD2	2.20	0.41
1:C:264:GLN:HB3	1:C:305:MET:HE2	2.01	0.41
1:D:635:THR:C	1:D:639:GLN:HE21	2.28	0.41
1:A:133:GLY:O	1:A:134:ASP:C	2.64	0.41
1:C:258:ASN:O	1:C:259:TYR:O	2.38	0.41
1:A:340:PHE:O	1:A:393:LYS:NZ	2.42	0.41
1:A:676:LYS:H	1:A:676:LYS:HG3	1.66	0.41
1:B:208:ASN:HD22	1:B:216:ASN:ND2	2.17	0.41
1:B:305:MET:HE2	1:B:309:ARG:HG3	2.03	0.41
1:B:477:TYR:CZ	1:B:487:ILE:HD11	2.55	0.41
1:C:64:ASN:ND2	1:C:79:TYR:H	2.17	0.41
1:C:138:HIS:CD2	1:C:140:PHE:CD2	3.09	0.41
1:C:203:MET:CE	1:C:239:MET:HE1	2.50	0.41
1:C:206:ILE:O	1:C:259:TYR:CD1	2.74	0.41
1:D:29:LYS:HD3	1:D:29:LYS:N	2.33	0.41
1:D:712:ARG:HA	1:D:715:MET:SD	2.60	0.41
1:A:405:LYS:CE	1:A:570:ASP:OD1	2.68	0.41
1:B:343:ARG:O	1:B:344:ASP:HB3	2.20	0.41
1:D:26:GLU:HG2	1:D:27:LEU:O	2.21	0.41
1:C:268:SER:O	1:C:274:PHE:HD2	2.04	0.41
1:D:689:GLU:OE2	1:D:692:ARG:NH2	2.53	0.41
1:A:80:LEU:N	1:A:80:LEU:HD22	2.34	0.41
1:A:110:ILE:CD1	3:A:2004:HOH:O	2.68	0.41
1:A:378:ARG:CZ	1:A:380:LEU:HD11	2.50	0.41
1:A:513:CYS:SG	1:A:565:LEU:HG	2.61	0.41
1:B:376:CYS:C	1:B:377:HIS:CD2	2.98	0.41
1:C:3:ALA:O	1:C:7:TYR:HB2	2.20	0.41
1:C:20:GLU:C	1:C:21:VAL:HG23	2.46	0.41
1:C:199:SER:O	1:C:200:ASN:C	2.63	0.41
1:C:231:ARG:O	1:C:232:TYR:C	2.63	0.41
1:C:573:TYR:O	1:C:574:GLU:C	2.63	0.41
1:D:31:TYR:CD2	1:D:31:TYR:C	2.98	0.41
1:D:349:ALA:O	1:D:350:ILE:C	2.62	0.41
1:A:138:HIS:HD2	1:A:140:PHE:H	1.68	0.41
1:A:210:LYS:HE2	1:A:255:GLU:O	2.21	0.41
1:C:81:HIS:CE1	1:C:84:ALA:H	2.39	0.41
1:C:82:GLU:HB3	1:C:83:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:LEU:HD23	1:C:279:LEU:CD2	2.50	0.41
1:C:293:SER:N	1:C:294:PRO:CD	2.84	0.41
1:C:652:ASN:HD22	1:C:652:ASN:HA	1.71	0.41
1:D:59:LEU:HB3	1:D:60:PRO:HD2	2.03	0.41
1:D:133:GLY:C	1:D:135:MET:N	2.79	0.41
1:A:344:ASP:O	1:A:345:SER:C	2.64	0.40
1:B:572:VAL:CG1	1:B:632:HIS:HD2	2.33	0.40
1:C:212:THR:HG23	1:C:256:GLU:OE1	2.20	0.40
1:C:283:ASN:HD21	1:C:294:PRO:HG3	1.85	0.40
1:C:746:LYS:HB3	1:C:747:THR:HG23	2.03	0.40
1:D:205:SER:HA	1:D:260:HIS:HB2	2.03	0.40
1:D:453:CYS:HB3	1:D:640:PHE:CE1	2.56	0.40
1:C:120:GLY:O	1:C:122:ASP:N	2.55	0.40
1:C:257:ARG:HB3	1:C:263:TYR:CE2	2.56	0.40
1:D:512:GLU:OE2	1:D:526:LYS:NZ	2.51	0.40
1:A:700:SER:O	1:A:701:ARG:HG3	2.21	0.40
1:B:192:VAL:O	1:B:193:GLU:C	2.64	0.40
1:B:463:GLN:HB2	1:B:492:ASN:HD21	1.86	0.40
1:C:17:ASP:O	1:C:21:VAL:CA	2.70	0.40
1:C:414:TRP:CZ2	1:C:418:HIS:NE2	2.90	0.40
1:D:398:ASN:HD22	1:D:398:ASN:N	2.18	0.40
1:A:157:GLN:HB2	1:A:433:ILE:HG23	2.04	0.40
1:B:340:PHE:CE1	1:B:396:ALA:HB1	2.56	0.40
1:C:67:ILE:HD11	1:C:760:GLU:OE2	2.20	0.40
1:C:94:ILE:HD11	1:C:673:PHE:HB3	2.03	0.40
1:D:530:THR:O	1:D:534:LYS:HD3	2.21	0.40
1:B:493:GLN:HE21	1:B:497:ASN:HD21	1.68	0.40
1:B:628:THR:O	1:B:632:HIS:CE1	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	714/766 (93%)	659 (92%)	43 (6%)	12 (2%)	7	19
1	B	709/766 (93%)	648 (91%)	51 (7%)	10 (1%)	9	23
1	C	715/766 (93%)	606 (85%)	81 (11%)	28 (4%)	2	5
1	D	707/766 (92%)	584 (83%)	92 (13%)	31 (4%)	2	4
All	All	2845/3064 (93%)	2497 (88%)	267 (9%)	81 (3%)	4	9

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	10	TYR
1	A	586	PHE
1	B	723	ASP
1	C	122	ASP
1	C	179	TYR
1	C	258	ASN
1	C	259	TYR
1	C	282	ALA
1	C	383	ALA
1	C	671	PHE
1	D	186	SER
1	D	297	ASP
1	D	344	ASP
1	D	348	CYS
1	D	394	LEU
1	D	395	HIS
1	D	583	SER
1	D	671	PHE
1	A	260	HIS
1	A	671	PHE
1	B	4	SER
1	B	671	PHE
1	C	35	ASP
1	C	94	ILE
1	C	180	PHE
1	C	214	ASN
1	C	277	LEU
1	D	114	GLU
1	D	134	ASP
1	D	165	SER
1	D	273	GLU
1	D	357	LEU

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Mol	Chain	Res	Type
1	A	4	SER
1	A	26	GLU
1	A	38	LEU
1	A	57	LYS
1	A	555	ASP
1	B	55	LYS
1	B	66	ASP
1	C	121	GLU
1	D	26	GLU
1	D	351	PRO
1	D	356	PRO
1	D	398	ASN
1	D	661	CYS
1	A	384	THR
1	B	33	PRO
1	B	35	ASP
1	B	271	LEU
1	B	533	ASN
1	C	5	GLU
1	C	21	VAL
1	C	52	LEU
1	C	78	SER
1	C	130	GLN
1	C	272	PRO
1	D	116	LEU
1	D	130	GLN
1	D	183	VAL
1	D	259	TYR
1	D	555	ASP
1	A	583	SER
1	C	66	ASP
1	C	230	LYS
1	C	318	SER
1	D	237	ALA
1	D	282	ALA
1	B	724	ARG
1	C	114	GLU
1	C	351	PRO
1	C	555	ASP
1	D	33	PRO
1	D	272	PRO
1	D	306	VAL

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Mol	Chain	Res	Type
1	D	338	VAL
1	D	350	ILE
1	D	18	PRO
1	C	65	PRO
1	C	124	ILE
1	C	687	VAL

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	605/672 (90%)	523 (86%)	82 (14%)	3	9
1	B	599/672 (89%)	523 (87%)	76 (13%)	4	11
1	C	589/672 (88%)	502 (85%)	87 (15%)	3	8
1	D	553/672 (82%)	459 (83%)	94 (17%)	2	6
All	All	2346/2688 (87%)	2007 (86%)	339 (14%)	3	8

All (339) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	5	GLU
1	A	15	ILE
1	A	19	GLU
1	A	26	GLU
1	A	27	LEU
1	A	32	LYS
1	A	35	ASP
1	A	36	LYS
1	A	37	VAL
1	A	38	LEU
1	A	41	ARG
1	A	49	GLU
1	A	52	LEU
1	A	58	GLU

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Mol	Chain	Res	Type
1	A	62	LEU
1	A	71	GLU
1	A	78	SER
1	A	105	ILE
1	A	114	GLU
1	A	128	SER
1	A	135	MET
1	A	139	ILE
1	A	152	ARG
1	A	160	ILE
1	A	191	ASN
1	A	210	LYS
1	A	212	THR
1	A	233	ARG
1	A	235	ILE
1	A	240	ARG
1	A	247	SER
1	A	257	ARG
1	A	261	ILE
1	A	271	LEU
1	A	272	PRO
1	A	276	THR
1	A	277	LEU
1	A	278	ARG
1	A	281	ASN
1	A	289	LYS
1	A	293	SER
1	A	299	ILE
1	A	303	LYS
1	A	322	GLN
1	A	350	ILE
1	A	355	ASP
1	A	359	ILE
1	A	364	MET
1	A	368	TYR
1	A	378	ARG
1	A	380	LEU
1	A	384	THR
1	A	389	LYS
1	A	425	SER
1	A	429	GLN
1	A	441	PHE

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Mol	Chain	Res	Type
1	A	443	THR
1	A	460	LYS
1	A	464	GLN
1	A	471	LYS
1	A	540	LYS
1	A	543	LEU
1	A	551	LYS
1	A	565	LEU
1	A	572	VAL
1	A	575	GLU
1	A	583	SER
1	A	587	LYS
1	A	588	LEU
1	A	632	HIS
1	A	646	LEU
1	A	655	THR
1	A	676	LYS
1	A	683	ARG
1	A	691	ILE
1	A	712	ARG
1	A	715	MET
1	A	716	LYS
1	A	724	ARG
1	A	741	LYS
1	A	748	LYS
1	B	4	SER
1	B	8	THR
1	B	19	GLU
1	B	20	GLU
1	B	36	LYS
1	B	39	GLN
1	B	40	LEU
1	B	41	ARG
1	B	42	LEU
1	B	47	ASP
1	B	51	CYS
1	B	69	VAL
1	B	86	LEU
1	B	94	ILE
1	B	110	ILE
1	B	115	GLN
1	B	123	ILE

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Mol	Chain	Res	Type
1	B	148	LYS
1	B	149	GLN
1	B	153	ASP
1	B	169	LYS
1	B	191	ASN
1	B	210	LYS
1	B	211	THR
1	B	212	THR
1	B	219	ARG
1	B	235	ILE
1	B	244	LEU
1	B	247	SER
1	B	276	THR
1	B	277	LEU
1	B	289	LYS
1	B	315	LEU
1	B	327	ARG
1	B	337	ASN
1	B	344	ASP
1	B	346	ASP
1	B	378	ARG
1	B	380	LEU
1	B	382	THR
1	B	389	LYS
1	B	393	LYS
1	B	425	SER
1	B	428	LYS
1	B	439	TYR
1	B	443	THR
1	B	446	ILE
1	B	492	ASN
1	B	506	LEU
1	B	515	MET
1	B	522	THR
1	B	540	LYS
1	B	543	LEU
1	B	544	SER
1	B	551	LYS
1	B	577	ILE
1	B	585	LYS
1	B	586	PHE
1	B	629	SER

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Mol	Chain	Res	Type
1	B	646	LEU
1	B	662	ILE
1	B	663	LYS
1	B	676	LYS
1	B	682	LEU
1	B	701	ARG
1	B	705	GLN
1	B	706	GLU
1	B	714	LEU
1	B	715	MET
1	B	716	LYS
1	B	723	ASP
1	B	725	LYS
1	B	739	LYS
1	B	740	ASP
1	B	746	LYS
1	B	755	GLN
1	C	12	ARG
1	C	19	GLU
1	C	36	LYS
1	C	47	ASP
1	C	52	LEU
1	C	53	ASP
1	C	56	THR
1	C	67	ILE
1	C	73	ASP
1	C	75	THR
1	C	80	LEU
1	C	82	GLU
1	C	85	VAL
1	C	89	LEU
1	C	115	GLN
1	C	122	ASP
1	C	125	ASN
1	C	132	MET
1	C	134	ASP
1	C	144	GLU
1	C	145	GLU
1	C	164	GLU
1	C	165	SER
1	C	174	LYS
1	C	177	MET

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Mol	Chain	Res	Type
1	C	193	GLU
1	C	210	LYS
1	C	213	ARG
1	C	215	ASP
1	C	217	SER
1	C	218	SER
1	C	219	ARG
1	C	229	ASP
1	C	230	LYS
1	C	241	THR
1	C	254	GLU
1	C	271	LEU
1	C	276	THR
1	C	277	LEU
1	C	279	LEU
1	C	283	ASN
1	C	300	ASP
1	C	313	THR
1	C	315	LEU
1	C	323	MET
1	C	327	ARG
1	C	337	ASN
1	C	342	SER
1	C	344	ASP
1	C	358	THR
1	C	367	ASP
1	C	379	LYS
1	C	394	LEU
1	C	418	HIS
1	C	421	LYS
1	C	423	LEU
1	C	429	GLN
1	C	438	ILE
1	C	445	GLU
1	C	458	ASN
1	C	471	LYS
1	C	479	LYS
1	C	486	LEU
1	C	502	LYS
1	C	525	GLN
1	C	526	LYS
1	C	543	LEU

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Mol	Chain	Res	Type
1	C	571	THR
1	C	577	ILE
1	C	583	SER
1	C	584	LYS
1	C	591	GLU
1	C	662	ILE
1	C	666	ASP
1	C	676	LYS
1	C	688	LEU
1	C	691	ILE
1	C	714	LEU
1	C	716	LYS
1	C	722	SER
1	C	724	ARG
1	C	725	LYS
1	C	729	LYS
1	C	741	LYS
1	C	746	LYS
1	C	762	ILE
1	C	763	ARG
1	D	19	GLU
1	D	20	GLU
1	D	23	LYS
1	D	29	LYS
1	D	36	LYS
1	D	38	LEU
1	D	42	LEU
1	D	47	ASP
1	D	53	ASP
1	D	67	ILE
1	D	71	GLU
1	D	80	LEU
1	D	89	LEU
1	D	90	LYS
1	D	96	SER
1	D	105	ILE
1	D	125	ASN
1	D	128	SER
1	D	131	ASN
1	D	132	MET
1	D	135	MET
1	D	136	ASP

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Mol	Chain	Res	Type
1	D	139	ILE
1	D	142	VAL
1	D	158	SER
1	D	161	VAL
1	D	164	GLU
1	D	170	THR
1	D	186	SER
1	D	191	ASN
1	D	192	VAL
1	D	200	ASN
1	D	231	ARG
1	D	233	ARG
1	D	235	ILE
1	D	238	ASN
1	D	247	SER
1	D	250	VAL
1	D	252	GLN
1	D	268	SER
1	D	271	LEU
1	D	275	LYS
1	D	276	THR
1	D	277	LEU
1	D	288	THR
1	D	293	SER
1	D	297	ASP
1	D	313	THR
1	D	315	LEU
1	D	320	SER
1	D	327	ARG
1	D	332	ILE
1	D	345	SER
1	D	348	CYS
1	D	351	PRO
1	D	354	HIS
1	D	355	ASP
1	D	357	LEU
1	D	362	ASP
1	D	376	CYS
1	D	380	LEU
1	D	382	THR
1	D	387	TYR
1	D	393	LYS

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Mol	Chain	Res	Type
1	D	405	LYS
1	D	406	HIS
1	D	420	ASN
1	D	439	TYR
1	D	448	SER
1	D	467	MET
1	D	478	MET
1	D	488	ASP
1	D	540	LYS
1	D	551	LYS
1	D	556	LYS
1	D	571	THR
1	D	574	GLU
1	D	581	LYS
1	D	589	LEU
1	D	649	GLU
1	D	661	CYS
1	D	662	ILE
1	D	677	ARG
1	D	683	ARG
1	D	692	ARG
1	D	700	SER
1	D	701	ARG
1	D	709	SER
1	D	712	ARG
1	D	714	LEU
1	D	731	VAL
1	D	740	ASP
1	D	749	ILE
1	D	756	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	87	HIS
1	A	88	ASN
1	A	138	HIS
1	A	157	GLN
1	A	191	ASN
1	A	216	ASN
1	A	260	HIS

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Mol	Chain	Res	Type
1	A	281	ASN
1	A	283	ASN
1	A	310	GLN
1	A	337	ASN
1	A	413	ASN
1	A	464	GLN
1	A	493	GLN
1	A	497	ASN
1	A	525	GLN
1	A	529	ASN
1	A	533	ASN
1	A	560	GLN
1	A	639	GLN
1	A	726	GLN
1	A	743	GLN
1	B	87	HIS
1	B	131	ASN
1	B	138	HIS
1	B	216	ASN
1	B	252	GLN
1	B	260	HIS
1	B	264	GLN
1	B	283	ASN
1	B	290	GLN
1	B	337	ASN
1	B	377	HIS
1	B	398	ASN
1	B	410	ASN
1	B	418	HIS
1	B	430	HIS
1	B	466	ASN
1	B	468	HIS
1	B	492	ASN
1	B	497	ASN
1	B	576	GLN
1	B	642	ASN
1	B	705	GLN
1	B	726	GLN
1	C	64	ASN
1	C	88	ASN
1	C	115	GLN
1	C	200	ASN

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Mol	Chain	Res	Type
1	C	286	HIS
1	C	310	GLN
1	C	322	GLN
1	C	334	HIS
1	C	337	ASN
1	C	373	HIS
1	C	398	ASN
1	C	406	HIS
1	C	410	ASN
1	C	420	ASN
1	C	424	HIS
1	C	462	GLN
1	C	463	GLN
1	C	466	ASN
1	C	468	HIS
1	C	481	GLN
1	C	493	GLN
1	C	497	ASN
1	C	576	GLN
1	C	652	ASN
1	D	125	ASN
1	D	131	ASN
1	D	191	ASN
1	D	216	ASN
1	D	238	ASN
1	D	252	GLN
1	D	264	GLN
1	D	310	GLN
1	D	334	HIS
1	D	377	HIS
1	D	398	ASN
1	D	406	HIS
1	D	420	ASN
1	D	424	HIS
1	D	463	GLN
1	D	466	ASN
1	D	493	GLN
1	D	497	ASN
1	D	525	GLN
1	D	531	HIS
1	D	639	GLN
1	D	665	ASN

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Mol	Chain	Res	Type
1	D	717	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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1767	-	4,4,4	0.43	0	6,6,6	0.24	0
2	SO4	D	1767	-	4,4,4	0.56	0	6,6,6	0.60	0
2	SO4	B	1764	-	4,4,4	0.55	0	6,6,6	0.73	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1767	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	722/766 (94%)	0.07	18 (2%) 58 55	22, 41, 64, 72	0
1	B	719/766 (93%)	0.19	15 (2%) 63 61	25, 46, 66, 74	0
1	C	723/766 (94%)	0.51	38 (5%) 32 28	23, 55, 69, 80	0
1	D	717/766 (93%)	0.73	56 (7%) 19 16	23, 60, 75, 82	0
All	All	2881/3064 (94%)	0.37	127 (4%) 39 35	22, 50, 71, 82	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	344	ASP	5.5
1	A	41	ARG	4.6
1	D	54	PRO	4.1
1	B	28	LEU	3.9
1	C	52	LEU	3.9
1	B	32	LYS	3.8
1	C	2	ALA	3.7
1	D	5	GLU	3.7
1	D	261	ILE	3.6
1	A	28	LEU	3.6
1	D	42	LEU	3.6
1	D	52	LEU	3.4
1	C	384	THR	3.4
1	A	54	PRO	3.3
1	B	54	PRO	3.3
1	C	3	ALA	3.3
1	B	764	ALA	3.2
1	D	274	PHE	3.1
1	B	50	TYR	3.1
1	D	198	ALA	3.1
1	C	296	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	187	ALA	3.0
1	B	57	LYS	2.9
1	D	381	ALA	2.9
1	D	296	ILE	2.9
1	B	51	CYS	2.9
1	C	383	ALA	2.9
1	D	298	GLY	2.9
1	C	326	PHE	2.9
1	C	69	VAL	2.8
1	A	56	THR	2.8
1	D	339	GLU	2.8
1	C	55	LYS	2.8
1	A	2	ALA	2.8
1	C	317	ILE	2.8
1	D	319	ASP	2.8
1	D	234	ILE	2.7
1	D	483	PRO	2.7
1	D	273	GLU	2.7
1	C	594	GLN	2.7
1	B	48	LEU	2.7
1	C	669	PHE	2.7
1	D	33	PRO	2.7
1	C	180	PHE	2.6
1	B	56	THR	2.6
1	C	717	GLN	2.6
1	D	268	SER	2.6
1	D	192	VAL	2.6
1	D	328	ILE	2.5
1	C	57	LYS	2.5
1	C	103	CYS	2.5
1	C	259	TYR	2.5
1	C	333	LEU	2.5
1	C	54	PRO	2.5
1	C	766	LYS	2.5
1	D	585	LYS	2.5
1	B	42	LEU	2.4
1	D	6	LEU	2.4
1	A	34	GLY	2.4
1	C	352	PRO	2.4
1	C	232	TYR	2.4
1	A	766	LYS	2.4
1	C	37	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	28	LEU	2.4
1	C	175	TYR	2.4
1	D	307	ASN	2.4
1	D	334	HIS	2.4
1	D	28	LEU	2.4
1	A	765	ASP	2.4
1	C	229	ASP	2.4
1	D	134	ASP	2.3
1	A	40	LEU	2.3
1	D	271	LEU	2.3
1	C	34	GLY	2.3
1	D	107	LEU	2.3
1	C	56	THR	2.3
1	C	184	SER	2.3
1	D	338	VAL	2.3
1	D	353	LYS	2.2
1	D	39	GLN	2.2
1	D	265	LEU	2.2
1	B	151	ALA	2.2
1	D	57	LYS	2.2
1	D	359	ILE	2.2
1	D	127	TYR	2.2
1	D	309	ARG	2.2
1	C	346	ASP	2.2
1	D	53	ASP	2.2
1	A	37	VAL	2.2
1	D	132	MET	2.2
1	D	41	ARG	2.2
1	C	665	ASN	2.2
1	A	543	LEU	2.2
1	D	383	ALA	2.2
1	C	428	LYS	2.2
1	D	135	MET	2.2
1	D	360	PHE	2.2
1	B	76	ALA	2.1
1	A	55	LYS	2.1
1	A	62	LEU	2.1
1	D	478	MET	2.1
1	D	341	ALA	2.1
1	C	8	THR	2.1
1	D	382	THR	2.1
1	D	482	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	720	VAL	2.1
1	A	5	GLU	2.1
1	C	19	GLU	2.1
1	C	41	ARG	2.1
1	A	57	LYS	2.1
1	D	387	TYR	2.1
1	B	37	VAL	2.1
1	C	47	ASP	2.0
1	D	343	ARG	2.0
1	D	367	ASP	2.0
1	C	33	PRO	2.0
1	D	272	PRO	2.0
1	A	6	LEU	2.0
1	A	52	LEU	2.0
1	A	645	HIS	2.0
1	C	20	GLU	2.0
1	D	146	ALA	2.0
1	D	151	ALA	2.0
1	D	740	ASP	2.0
1	D	352	PRO	2.0
1	B	68	LEU	2.0
1	D	50	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	1764	5/5	0.71	0.18	70,71,72,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	1767	5/5	0.73	0.17	72,72,73,76	0
2	SO4	A	1767	5/5	0.81	0.18	71,71,72,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.