



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:00 PM UTC

PDB ID : 4F5U / pdb_00004f5u
Title : Crystal structure of Equine Serum Albumin at 2.04 resolution
Authors : Bujacz, A.; Bujacz, G.
Deposited on : 2012-05-13
Resolution : 2.04 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

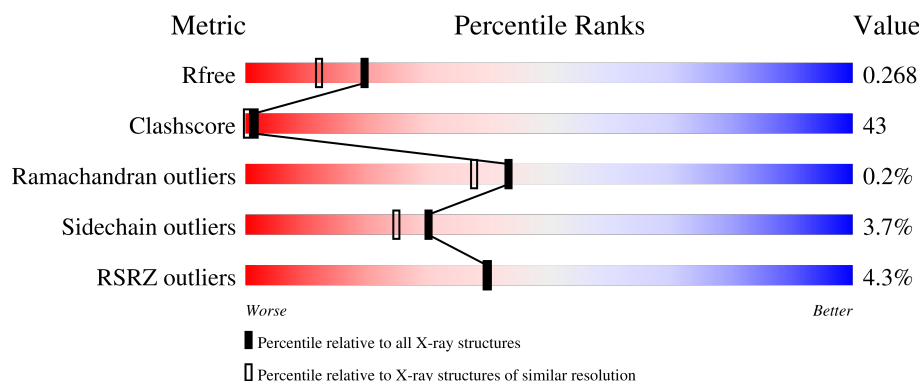
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	583	

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
2	MLI	A	601	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MLI	A	603	-	-	X	-
2	MLI	A	606	-	-	X	-
3	SIN	A	607	-	-	X	-
4	LMR	A	608	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5063 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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	583	4659	2948	779	897	35	0	9	0

- Molecule 2 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



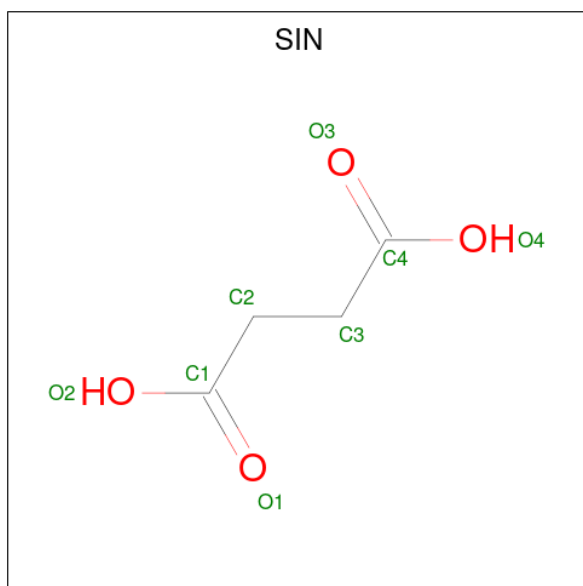
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	7	3	4	0	0
2	A	1	7	3	4	0	0
2	A	1	7	3	4	0	0
2	A	1	7	3	4	0	0
2	A	1	7	3	4	0	0

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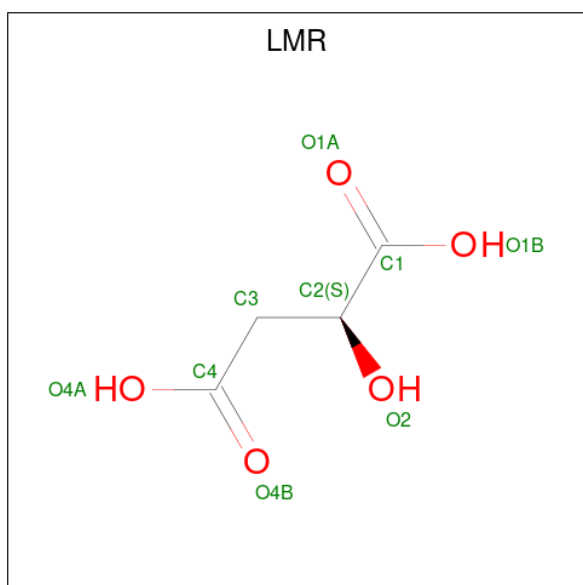
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 3 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: C₄H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	4	5		

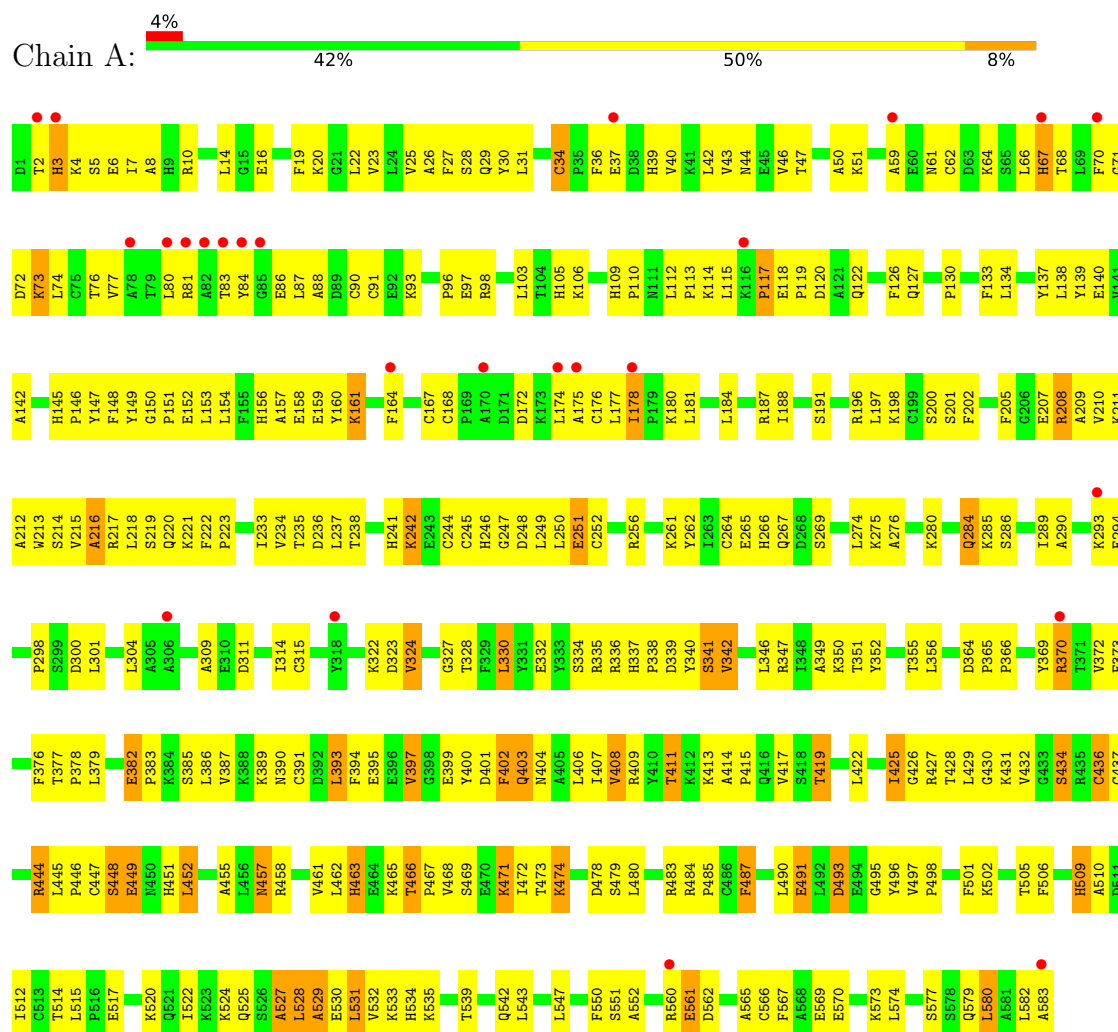
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	345	Total	O	0	0
			345	345		

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: Serum albumin



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	89.25Å 89.25Å 134.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.04 50.00 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.04) 99.8 (50.00-2.04)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.196 , 0.243 0.217 , 0.268	Depositor DCC
R_{free} test set	1211 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.053 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5063	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: SIN, MLI, LMR

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	1.36	22/4783 (0.5%)	1.32	42/6451 (0.7%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	408	VAL	CA-CB	-5.95	1.47	1.54
1	A	457	ASN	N-CA	-5.88	1.38	1.46
1	A	109	HIS	N-CA	-5.76	1.40	1.46
1	A	245	CYS	CA-C	-5.69	1.45	1.52
1	A	236	ASP	CA-C	-5.69	1.45	1.52
1	A	419	THR	N-CA	-5.48	1.40	1.46
1	A	474	LYS	N-CA	-5.46	1.39	1.46
1	A	342	VAL	CA-CB	-5.31	1.48	1.54
1	A	436	CYS	CA-C	-5.31	1.45	1.52
1	A	509	HIS	CA-C	-5.28	1.46	1.52
1	A	528	LEU	C-O	-5.25	1.18	1.24
1	A	506	PHE	CA-C	-5.23	1.45	1.52
1	A	403	GLN	CA-C	-5.22	1.46	1.52
1	A	448	SER	CA-C	-5.22	1.46	1.52
1	A	222	PHE	CA-C	-5.17	1.46	1.52
1	A	284	GLN	C-O	-5.14	1.18	1.24
1	A	463	HIS	N-CA	-5.10	1.39	1.46
1	A	449	GLU	N-CA	-5.10	1.39	1.46
1	A	212	ALA	N-CA	-5.06	1.40	1.46
1	A	444	ARG	C-O	-5.05	1.18	1.24
1	A	222	PHE	CA-CB	-5.04	1.47	1.53
1	A	487	PHE	C-O	-5.00	1.18	1.24

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	LEU	N-CA-C	-7.73	102.94	111.36
1	A	382	GLU	CA-C-N	-7.41	111.34	119.19
1	A	382	GLU	C-N-CA	-7.41	111.34	119.19
1	A	269	SER	N-CA-C	-7.27	103.50	112.88
1	A	212	ALA	N-CA-C	-6.94	103.80	111.36
1	A	330	LEU	N-CA-C	-6.86	103.88	111.36
1	A	552	ALA	N-CA-C	-6.83	103.91	111.36
1	A	269	SER	CA-C-N	-6.78	116.33	122.97
1	A	269	SER	C-N-CA	-6.78	116.33	122.97
1	A	514	THR	N-CA-C	-6.73	105.10	113.38
1	A	520	LYS	N-CA-C	-6.42	104.29	111.28
1	A	178	ILE	CA-C-N	-6.41	111.86	118.85
1	A	178	ILE	C-N-CA	-6.41	111.86	118.85
1	A	71	GLY	N-CA-C	-6.41	105.07	112.50
1	A	242	LYS	N-CA-C	-6.39	104.23	111.07
1	A	338	PRO	N-CA-C	-6.12	106.50	114.03
1	A	68	THR	N-CA-C	-6.11	104.53	111.07
1	A	327	GLY	N-CA-C	-5.98	105.56	112.50
1	A	491	GLU	N-CA-C	-5.92	100.58	108.34
1	A	471	LYS	N-CA-C	-5.89	104.45	111.69
1	A	403	GLN	N-CA-C	-5.86	104.90	111.28
1	A	531	LEU	N-CA-C	-5.82	104.93	111.28
1	A	565	ALA	N-CA-C	-5.82	104.93	111.28
1	A	466	THR	CA-C-N	5.72	125.91	119.90
1	A	466	THR	C-N-CA	5.72	125.91	119.90
1	A	529	ALA	N-CA-C	-5.67	105.00	111.07
1	A	216	ALA	N-CA-C	-5.62	105.05	111.07
1	A	426	GLY	N-CA-C	-5.61	105.59	112.77
1	A	209	ALA	N-CA-C	-5.54	104.88	111.69
1	A	341	SER	N-CA-C	-5.49	103.13	110.55
1	A	197	LEU	N-CA-C	-5.47	105.32	111.28
1	A	251	GLU	N-CA-C	-5.41	105.46	111.36
1	A	235	THR	N-CA-C	-5.41	105.30	111.14
1	A	411	THR	N-CA-C	-5.40	105.56	111.82
1	A	474	LYS	N-CA-C	-5.33	105.37	111.07
1	A	402	PHE	N-CA-C	-5.27	105.62	111.36
1	A	324	VAL	N-CA-C	-5.21	106.61	111.45
1	A	527	ALA	N-CA-C	-5.13	105.69	111.28
1	A	187	ARG	N-CA-C	-5.09	105.81	111.36
1	A	461	VAL	N-CA-C	-5.04	105.63	110.72
1	A	109	HIS	CA-C-N	-5.04	114.63	119.87
1	A	109	HIS	C-N-CA	-5.04	114.63	119.87

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	4659	0	4594	398	0
2	A	42	0	12	21	0
3	A	8	0	4	6	0
4	A	9	0	4	13	0
5	A	345	0	0	39	0
All	All	5063	0	4614	405	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 43.

All (405) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ARG:HD2	1:A:370:ARG:O	1.39	1.21
1:A:425:ILE:HD12	5:A:1039:HOH:O	1.46	1.13
1:A:391:CYS:O	1:A:395:GLU:HG2	1.49	1.11
1:A:560:ARG:HD2	1:A:562:ASP:H	1.08	1.09
1:A:409:ARG:HH11	2:A:603:MLI:H11	0.91	1.05
1:A:409:ARG:NH1	2:A:603:MLI:H11	1.71	1.04
1:A:457:ASN:HD22	1:A:483:ARG:HH12	1.06	1.03
1:A:267:GLN:HE22	1:A:275:LYS:HA	1.26	1.00
1:A:134:LEU:CD1	1:A:161:LYS:HD3	1.92	0.99
1:A:10:ARG:HG3	1:A:66:LEU:HD11	1.46	0.94
1:A:66:LEU:HB3	1:A:70:PHE:HE1	1.32	0.92
1:A:66:LEU:HB3	1:A:70:PHE:CE1	2.04	0.92
1:A:31:LEU:O	1:A:39:HIS:CE1	2.23	0.91
1:A:409:ARG:HH11	2:A:603:MLI:C1	1.82	0.91
1:A:560:ARG:HD2	1:A:562:ASP:N	1.86	0.90
1:A:237:LEU:HD13	3:A:607:SIN:H22	1.53	0.89
1:A:134:LEU:HD11	1:A:161:LYS:HD3	1.53	0.89
1:A:397:VAL:HG13	1:A:401:ASP:HB2	1.52	0.89
1:A:397:VAL:HG13	1:A:401:ASP:CB	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:HIS:CD2	1:A:248:ASP:OD1	2.26	0.88
1:A:31:LEU:O	1:A:39:HIS:HE1	1.58	0.84
1:A:208:ARG:HD2	5:A:746:HOH:O	1.77	0.84
1:A:40:VAL:O	1:A:43:VAL:HG12	1.79	0.83
1:A:351:THR:OG1	1:A:379:LEU:HD11	1.79	0.82
1:A:134:LEU:HD11	1:A:161:LYS:CD	2.10	0.81
1:A:560:ARG:CD	1:A:562:ASP:H	1.92	0.81
1:A:66:LEU:CB	2:A:601:MLI:H12	2.11	0.80
1:A:370:ARG:O	1:A:370:ARG:CD	2.28	0.80
1:A:29:GLN:HG3	1:A:142:ALA:HB1	1.62	0.79
1:A:26:ALA:O	1:A:30:TYR:HD2	1.65	0.77
1:A:382:GLU:OE2	1:A:386:LEU:HD12	1.84	0.77
1:A:417:VAL:CG2	1:A:472:ILE:HD11	2.14	0.77
1:A:493:ASP:OD2	1:A:493:ASP:N	2.19	0.76
1:A:66:LEU:HB3	2:A:601:MLI:H12	1.67	0.76
1:A:407:ILE:HD13	1:A:525:GLN:HB3	1.69	0.75
1:A:122:GLN:HB3	1:A:164:PHE:CE1	2.22	0.75
1:A:201:SER:HB3	2:A:606:MLI:H11	1.69	0.74
1:A:534:HIS:HD2	1:A:579:GLN:OE1	1.70	0.74
1:A:237:LEU:HD11	3:A:607:SIN:H31	1.70	0.74
1:A:465:LYS:HD3	1:A:466:THR:OG1	1.88	0.74
1:A:409:ARG:HG2	1:A:413:LYS:HE2	1.70	0.73
1:A:205:PHE:CD2	1:A:480:LEU:HD22	2.24	0.73
1:A:415:PRO:O	1:A:533:LYS:HE2	1.89	0.73
1:A:66:LEU:HD22	1:A:70:PHE:CZ	2.26	0.71
1:A:208:ARG:H	1:A:208:ARG:HE	1.35	0.71
1:A:207:GLU:H	1:A:208:ARG:HH21	1.36	0.71
1:A:246:HIS:HE1	5:A:796:HOH:O	1.73	0.71
1:A:407:ILE:CD1	1:A:525:GLN:HB3	2.20	0.71
1:A:103:LEU:O	1:A:106:LYS:HB2	1.91	0.70
1:A:406:LEU:HD13	1:A:429:LEU:HB3	1.73	0.70
1:A:46:VAL:HG23	1:A:73:LYS:HG3	1.74	0.69
1:A:198:LYS:CE	4:A:608:LMR:O4B	2.41	0.69
1:A:352:TYR:CE2	1:A:356:LEU:HD11	2.27	0.69
1:A:213:TRP:HZ3	4:A:608:LMR:H3A	1.57	0.69
1:A:134:LEU:HD13	1:A:161:LYS:HD3	1.71	0.68
1:A:414:ALA:HB1	1:A:472:ILE:HD11	1.74	0.68
1:A:114:LYS:HD2	5:A:1038:HOH:O	1.93	0.68
1:A:213:TRP:HB2	2:A:606:MLI:H12	1.73	0.68
1:A:122:GLN:HB3	1:A:164:PHE:HE1	1.58	0.67
1:A:355:THR:HG21	1:A:372:VAL:HG23	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LYS:NZ	5:A:731:HOH:O	2.29	0.66
1:A:293[B]:LYS:H	1:A:293[B]:LYS:HD2	1.59	0.66
1:A:6:GLU:HG3	5:A:1036:HOH:O	1.95	0.66
1:A:31:LEU:CD2	1:A:87:LEU:CD1	2.73	0.66
1:A:341:SER:HB3	1:A:449:GLU:HB3	1.77	0.66
1:A:417:VAL:CG2	1:A:472:ILE:CD1	2.72	0.66
1:A:223:PRO:HA	1:A:335:ARG:HB2	1.78	0.66
1:A:198:LYS:HE3	4:A:608:LMR:O4B	1.96	0.66
1:A:207:GLU:HG2	1:A:211:LYS:HE3	1.76	0.66
1:A:406:LEU:HD13	1:A:429:LEU:CB	2.26	0.65
1:A:80:LEU:HD21	1:A:91:CYS:SG	2.36	0.65
1:A:267:GLN:HE22	1:A:275:LYS:CA	2.07	0.65
1:A:256:ARG:HD3	2:A:604:MLI:O8	1.96	0.65
1:A:201:SER:CB	2:A:606:MLI:H11	2.25	0.65
1:A:256:ARG:CZ	1:A:286:SER:HB3	2.26	0.65
1:A:370:ARG:HD2	1:A:370:ARG:C	2.20	0.64
1:A:465:LYS:CD	1:A:466:THR:OG1	2.45	0.64
1:A:127:GLN:NE2	1:A:168:CYS:HB3	2.13	0.64
1:A:130:PRO:O	1:A:134:LEU:HG	1.97	0.64
1:A:208:ARG:H	1:A:208:ARG:NE	1.95	0.64
1:A:409:ARG:NH1	2:A:603:MLI:C1	2.50	0.64
1:A:469:SER:HB3	1:A:472:ILE:HD12	1.80	0.64
1:A:40:VAL:HA	1:A:43:VAL:HG12	1.78	0.64
1:A:248:ASP:HB3	2:A:601:MLI:C3	2.28	0.64
1:A:115:LEU:HD11	1:A:140:GLU:HB3	1.79	0.64
1:A:40:VAL:O	1:A:43:VAL:CG1	2.46	0.63
1:A:167:CYS:HB2	1:A:177:LEU:HD13	1.79	0.63
1:A:304:LEU:HB3	1:A:373:PHE:CZ	2.33	0.63
1:A:304:LEU:HG	1:A:336:ARG:CZ	2.27	0.63
1:A:539:THR:OG1	1:A:542:GLN:HG3	1.97	0.63
4:A:608:LMR:C2	5:A:742:HOH:O	2.45	0.63
1:A:213:TRP:CZ3	4:A:608:LMR:H3A	2.33	0.63
1:A:40:VAL:C	1:A:43:VAL:HG12	2.23	0.63
1:A:67:HIS:HD2	1:A:248:ASP:OD1	1.80	0.63
1:A:262:TYR:O	1:A:266:HIS:HD2	1.82	0.62
1:A:293[B]:LYS:H	1:A:293[B]:LYS:CD	2.11	0.62
1:A:560:ARG:HD3	1:A:561:GLU:H	1.64	0.62
1:A:322:LYS:HE2	5:A:898:HOH:O	1.99	0.62
1:A:332:GLU:OE1	1:A:335:ARG:HD3	2.00	0.62
1:A:573:LYS:HG2	5:A:942:HOH:O	1.99	0.62
1:A:31:LEU:HD21	1:A:87:LEU:HD13	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HB2	2:A:601:MLI:H12	1.80	0.62
1:A:379:LEU:O	1:A:383:PRO:HD2	1.99	0.62
1:A:110:PRO:HD2	5:A:718:HOH:O	2.00	0.61
1:A:393:LEU:O	1:A:397:VAL:HB	2.00	0.61
1:A:397:VAL:HG13	1:A:401:ASP:HB3	1.83	0.61
1:A:583:ALA:HB2	5:A:781:HOH:O	2.00	0.61
1:A:117:PRO:O	1:A:119:PRO:HD3	2.01	0.60
1:A:22:LEU:HG	1:A:154:LEU:HD11	1.83	0.60
1:A:66:LEU:O	1:A:70:PHE:CD1	2.55	0.60
1:A:40:VAL:CA	1:A:43:VAL:HG12	2.31	0.60
1:A:172:ASP:OD1	1:A:175:ALA:HB3	2.02	0.60
4:A:608:LMR:H2	5:A:742:HOH:O	2.01	0.60
1:A:560:ARG:HG3	1:A:566:CYS:HB2	1.82	0.59
1:A:382:GLU:OE2	1:A:386:LEU:CD1	2.50	0.59
1:A:31:LEU:HD21	1:A:87:LEU:CD1	2.33	0.59
1:A:198:LYS:HE2	4:A:608:LMR:O4B	2.02	0.59
1:A:127:GLN:HE21	1:A:168:CYS:HB3	1.66	0.59
1:A:290:ALA:O	4:A:608:LMR:O1A	2.21	0.59
1:A:42:LEU:HD21	5:A:1025:HOH:O	2.02	0.59
1:A:248:ASP:HA	2:A:601:MLI:C2	2.32	0.59
1:A:145:HIS:NE2	5:A:1042:HOH:O	2.32	0.59
1:A:462:LEU:O	1:A:465:LYS:HD2	2.03	0.59
1:A:246:HIS:CE1	5:A:796:HOH:O	2.52	0.59
1:A:390:ASN:HD21	2:A:603:MLI:H12	1.69	0.58
1:A:117:PRO:HB2	1:A:178:ILE:HG12	1.85	0.58
1:A:176:CYS:O	1:A:180:LYS:HG2	2.03	0.58
1:A:81:ARG:HG2	1:A:88:ALA:HB2	1.84	0.58
1:A:280:LYS:HD2	1:A:284:GLN:NE2	2.18	0.58
1:A:7:ILE:HA	1:A:66:LEU:HD21	1.84	0.58
4:A:608:LMR:C1	5:A:742:HOH:O	2.51	0.58
1:A:280:LYS:HD2	1:A:284:GLN:HE21	1.69	0.58
1:A:379:LEU:O	1:A:383:PRO:CD	2.51	0.58
1:A:213:TRP:HZ3	4:A:608:LMR:C3	2.17	0.58
1:A:534:HIS:HB3	5:A:867:HOH:O	2.03	0.58
1:A:219:SER:HB2	1:A:334:SER:HB2	1.86	0.57
1:A:404:ASN:OD1	1:A:525:GLN:HG2	2.04	0.57
1:A:387:VAL:HG21	1:A:445:LEU:HA	1.86	0.57
1:A:517[B]:GLU:HG3	5:A:1002:HOH:O	2.03	0.57
1:A:28:SER:HB2	1:A:142:ALA:HB3	1.86	0.57
1:A:341:SER:CB	1:A:449:GLU:HB3	2.35	0.57
1:A:156:HIS:NE2	5:A:854:HOH:O	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ARG:CG	1:A:413:LYS:HE2	2.34	0.57
1:A:202:PHE:CZ	1:A:210:VAL:HG11	2.40	0.57
1:A:81:ARG:HG2	1:A:88:ALA:CB	2.35	0.57
1:A:47:THR:O	1:A:50:ALA:HB3	2.06	0.56
1:A:484:ARG:HB3	1:A:485:PRO:HD3	1.87	0.56
1:A:248:ASP:HB3	2:A:601:MLI:O9	2.05	0.56
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.45	0.56
1:A:201:SER:HB2	1:A:210:VAL:HG22	1.88	0.56
1:A:411:THR:HG23	1:A:422:LEU:HD13	1.87	0.56
1:A:84:TYR:HB2	1:A:87:LEU:HB2	1.87	0.56
1:A:385:SER:O	1:A:389:LYS:HG3	2.06	0.56
1:A:427:ARG:HD2	1:A:522:ILE:HG12	1.88	0.56
1:A:237:LEU:CD1	3:A:607:SIN:H31	2.36	0.55
1:A:40:VAL:HA	1:A:43:VAL:CG1	2.37	0.55
1:A:493:ASP:C	1:A:495:GLY:H	2.15	0.55
1:A:463:HIS:HE1	1:A:473:THR:OG1	1.90	0.55
1:A:417:VAL:HG23	1:A:472:ILE:HD11	1.88	0.55
1:A:248:ASP:HA	2:A:601:MLI:C1	2.36	0.55
1:A:324:VAL:O	1:A:328:THR:OG1	2.22	0.55
1:A:27:PHE:HE1	1:A:70:PHE:HB3	1.73	0.54
1:A:237:LEU:HD13	3:A:607:SIN:C2	2.33	0.54
1:A:251:GLU:HB2	2:A:601:MLI:O9	2.07	0.54
1:A:394:PHE:CZ	1:A:434:SER:HA	2.42	0.54
1:A:560:ARG:HD3	1:A:561:GLU:N	2.21	0.54
1:A:582:LEU:O	1:A:583:ALA:C	2.50	0.54
1:A:509:HIS:O	1:A:512:ILE:HG22	2.08	0.54
1:A:31:LEU:HD23	1:A:87:LEU:CD1	2.38	0.54
1:A:417:VAL:HG21	1:A:472:ILE:HD11	1.86	0.54
1:A:355:THR:CG2	1:A:372:VAL:HG23	2.37	0.53
1:A:133:PHE:HZ	1:A:164:PHE:CZ	2.26	0.53
2:A:606:MLI:O8	2:A:606:MLI:O6	2.23	0.53
1:A:37[B]:GLU:CD	1:A:37[B]:GLU:H	2.17	0.53
1:A:46:VAL:CG2	1:A:73:LYS:HG3	2.37	0.53
1:A:117:PRO:HD3	5:A:789:HOH:O	2.08	0.53
1:A:214:SER:HB2	1:A:234:VAL:HG13	1.91	0.53
1:A:304:LEU:HD21	1:A:332:GLU:HB3	1.91	0.52
1:A:138:LEU:HD23	1:A:153:LEU:HG	1.91	0.52
1:A:341:SER:HA	1:A:446:PRO:HA	1.92	0.52
1:A:417:VAL:HA	1:A:468:VAL:HG21	1.91	0.52
1:A:262:TYR:C	1:A:262:TYR:CD2	2.88	0.52
1:A:267:GLN:NE2	1:A:275:LYS:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:PRO:HB2	1:A:496:TYR:CZ	2.44	0.52
1:A:261:LYS:O	1:A:265:GLU:HG2	2.10	0.52
1:A:200:SER:CB	1:A:457:ASN:HD21	2.23	0.51
1:A:213:TRP:CD1	2:A:606:MLI:C3	2.93	0.51
1:A:242:LYS:O	1:A:246:HIS:CD2	2.63	0.51
2:A:601:MLI:O7	2:A:601:MLI:O8	2.25	0.51
1:A:77:VAL:HG22	1:A:80:LEU:HD13	1.91	0.51
1:A:352:TYR:CZ	1:A:356:LEU:HD11	2.45	0.51
1:A:72:ASP:O	1:A:76:THR:HG23	2.11	0.51
1:A:87:LEU:O	1:A:90:CYS:HB2	2.11	0.51
1:A:30:TYR:OH	1:A:247:GLY:HA3	2.10	0.50
1:A:84:TYR:CB	1:A:87:LEU:HB2	2.41	0.50
1:A:436:CYS:O	1:A:444:ARG:HG2	2.10	0.50
1:A:471:LYS:HD3	1:A:490:LEU:HD22	1.92	0.50
1:A:66:LEU:HD22	1:A:70:PHE:HZ	1.74	0.50
1:A:455:ALA:O	1:A:458:ARG:HB3	2.12	0.50
1:A:126:PHE:HB2	1:A:133:PHE:CD2	2.46	0.50
1:A:149:TYR:HB3	1:A:152:GLU:HB2	1.93	0.50
1:A:216:ALA:HB3	1:A:342:VAL:HG13	1.93	0.50
1:A:501:PHE:HB2	1:A:534:HIS:CE1	2.46	0.50
1:A:532:VAL:HG22	1:A:543:LEU:HD13	1.92	0.50
1:A:399:GLU:O	1:A:403:GLN:HG3	2.12	0.50
1:A:402:PHE:CD2	1:A:430:GLY:HA2	2.47	0.50
1:A:493:ASP:C	1:A:495:GLY:N	2.69	0.50
1:A:31:LEU:HD12	1:A:74:LEU:HD22	1.94	0.50
1:A:42:LEU:HD11	1:A:77:VAL:HG13	1.93	0.50
1:A:19:PHE:O	1:A:23:VAL:HG23	2.12	0.50
1:A:309:ALA:HB1	1:A:370:ARG:HD3	1.94	0.50
1:A:304:LEU:HB3	1:A:373:PHE:HZ	1.77	0.49
1:A:364:ASP:N	5:A:966:HOH:O	2.44	0.49
1:A:43:VAL:HG13	1:A:44:ASN:N	2.27	0.49
1:A:83:THR:HB	1:A:84:TYR:CE1	2.47	0.49
1:A:462:LEU:HA	1:A:465:LYS:HE3	1.94	0.49
1:A:284:GLN:HG3	5:A:801:HOH:O	2.12	0.49
1:A:330:LEU:HD13	1:A:349:ALA:HB2	1.94	0.49
1:A:31:LEU:CD2	1:A:87:LEU:HD12	2.43	0.49
1:A:332:GLU:O	1:A:335:ARG:HG2	2.12	0.49
1:A:118:GLU:N	1:A:122:GLN:OE1	2.45	0.49
1:A:465:LYS:C	1:A:467:PRO:HD3	2.38	0.49
1:A:201:SER:OG	1:A:480:LEU:HD21	2.12	0.49
1:A:151:PRO:HB2	1:A:256:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASP:HA	5:A:1001:HOH:O	2.13	0.48
1:A:220:GLN:O	1:A:223:PRO:HD3	2.13	0.48
1:A:293[A]:LYS:HD3	1:A:293[A]:LYS:HA	1.59	0.48
1:A:535:LYS:HG3	1:A:582:LEU:HB2	1.94	0.48
1:A:400:TYR:OH	1:A:524:LYS:HE2	2.13	0.48
1:A:457:ASN:HD22	1:A:483:ARG:NH1	1.91	0.48
1:A:339:ASP:O	1:A:446:PRO:HD3	2.13	0.48
1:A:86:GLU:HB2	1:A:105:HIS:CD2	2.48	0.48
1:A:213:TRP:HZ3	4:A:608:LMR:C4	2.27	0.48
1:A:215:VAL:HA	1:A:234:VAL:HG21	1.95	0.48
1:A:315:CYS:SG	1:A:365:PRO:HB3	2.54	0.48
1:A:478:ASP:O	1:A:479:SER:C	2.54	0.48
1:A:211:LYS:O	1:A:215:VAL:HG23	2.13	0.48
1:A:5:SER:HB3	1:A:8:ALA:HB3	1.96	0.48
1:A:505:THR:CG2	1:A:530:GLU:HG3	2.44	0.48
1:A:87:LEU:O	1:A:88:ALA:C	2.56	0.47
1:A:207:GLU:N	1:A:208:ARG:HE	2.11	0.47
1:A:427:ARG:HD2	1:A:522:ILE:CG1	2.45	0.47
1:A:137:TYR:HB2	1:A:160:TYR:CE2	2.50	0.47
1:A:264:CYS:HB3	5:A:897:HOH:O	2.14	0.47
1:A:66:LEU:CB	1:A:70:PHE:CE1	2.89	0.47
1:A:70:PHE:CZ	1:A:250:LEU:HD12	2.49	0.47
1:A:83:THR:HB	1:A:84:TYR:CD1	2.50	0.47
1:A:164:PHE:CZ	1:A:181:LEU:HD11	2.49	0.47
1:A:569:GLU:HG3	1:A:570[A]:GLU:HG2	1.97	0.47
1:A:36:PHE:HB2	1:A:139:TYR:CD2	2.50	0.47
1:A:534:HIS:CD2	1:A:579:GLN:OE1	2.59	0.47
1:A:218:LEU:HD13	1:A:233:ILE:HG22	1.97	0.47
1:A:156:HIS:ND1	1:A:159:GLU:OE2	2.39	0.46
1:A:365:PRO:HB2	1:A:366:PRO:HD3	1.97	0.46
1:A:351:THR:OG1	1:A:379:LEU:CD1	2.57	0.46
1:A:34:CYS:HB2	1:A:39:HIS:CE1	2.51	0.46
1:A:383:PRO:HB2	1:A:445:LEU:HD11	1.96	0.46
1:A:399:GLU:OE2	5:A:807:HOH:O	2.21	0.46
1:A:449:GLU:HG2	5:A:858:HOH:O	2.15	0.46
1:A:154:LEU:O	1:A:158:GLU:HG2	2.16	0.46
1:A:207:GLU:CG	1:A:211:LYS:HE3	2.45	0.46
1:A:406:LEU:HD23	1:A:406:LEU:HA	1.82	0.46
1:A:6:GLU:O	1:A:10:ARG:HG2	2.16	0.46
1:A:213:TRP:CD1	1:A:342:VAL:HG11	2.50	0.46
1:A:265:GLU:HB2	1:A:266:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:HIS:O	1:A:4:LYS:C	2.58	0.46
1:A:215:VAL:O	1:A:219:SER:OG	2.28	0.46
1:A:311:ASP:HB3	1:A:314:ILE:HG13	1.98	0.46
1:A:276:ALA:O	1:A:280:LYS:HG2	2.16	0.46
1:A:403:GLN:HG2	1:A:430:GLY:HA3	1.98	0.45
1:A:550:PHE:HA	1:A:574:LEU:HD21	1.97	0.45
1:A:36:PHE:HB2	1:A:139:TYR:CE2	2.51	0.45
1:A:497:VAL:O	1:A:498:PRO:C	2.59	0.45
1:A:515:LEU:HD23	1:A:515:LEU:HA	1.74	0.45
1:A:25:VAL:O	1:A:26:ALA:C	2.60	0.45
1:A:463:HIS:CE1	1:A:473:THR:OG1	2.69	0.45
1:A:134:LEU:HD11	1:A:161:LYS:HD2	1.94	0.45
1:A:370:ARG:CD	1:A:370:ARG:C	2.87	0.45
1:A:246:HIS:CG	5:A:962:HOH:O	2.69	0.45
1:A:298:PRO:HB2	1:A:300:ASP:OD1	2.15	0.45
1:A:347:ARG:HH22	1:A:449:GLU:CD	2.25	0.45
1:A:527:ALA:O	1:A:531:LEU:N	2.47	0.45
1:A:352:TYR:HE1	1:A:372:VAL:HG11	1.81	0.45
1:A:19:PHE:CD2	1:A:19:PHE:C	2.95	0.45
1:A:213:TRP:CE2	1:A:342:VAL:HG11	2.51	0.45
1:A:47:THR:O	1:A:51:LYS:HG3	2.17	0.45
1:A:112:LEU:O	1:A:113:PRO:C	2.56	0.45
1:A:577:SER:O	1:A:580:LEU:HB2	2.17	0.45
1:A:20:LYS:HG2	1:A:47:THR:OG1	2.17	0.45
1:A:29:GLN:HG2	1:A:146:PRO:HA	1.98	0.45
1:A:221:LYS:HA	1:A:294:GLU:HG2	1.98	0.45
1:A:90:CYS:HA	1:A:93:LYS:HD2	1.99	0.44
1:A:138:LEU:CD2	1:A:153:LEU:HG	2.46	0.44
1:A:149:TYR:CD2	1:A:152:GLU:HG2	2.53	0.44
1:A:207:GLU:O	1:A:211:LYS:HG3	2.16	0.44
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.74	0.44
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.80	0.44
1:A:27:PHE:CE1	1:A:70:PHE:HB3	2.53	0.44
1:A:74:LEU:O	1:A:77:VAL:HG22	2.16	0.44
1:A:249:LEU:HA	1:A:252:CYS:HB3	1.99	0.44
1:A:437:CYS:O	1:A:444:ARG:CZ	2.66	0.44
1:A:61:ASN:OD1	1:A:64:LYS:HE2	2.17	0.44
1:A:77:VAL:CG2	1:A:80:LEU:HD13	2.47	0.44
1:A:207:GLU:HG3	1:A:238:THR:CG2	2.48	0.44
1:A:355:THR:CB	1:A:372:VAL:HG23	2.48	0.44
1:A:419:THR:HG23	1:A:529:ALA:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ARG:O	1:A:431:LYS:HG3	2.17	0.44
1:A:493:ASP:HB2	1:A:496:TYR:H	1.83	0.44
1:A:93:LYS:HD3	1:A:97[A]:GLU:HG2	2.00	0.44
1:A:133:PHE:HZ	1:A:164:PHE:CE1	2.34	0.44
1:A:366:PRO:HA	1:A:369:TYR:CE1	2.52	0.44
1:A:138:LEU:HD21	1:A:157:ALA:HB2	2.00	0.44
1:A:217:ARG:HG2	4:A:608:LMR:H3A	2.00	0.44
1:A:241:HIS:NE2	5:A:871:HOH:O	2.36	0.44
1:A:264:CYS:SG	1:A:289:ILE:HD11	2.57	0.44
1:A:16:GLU:OE2	1:A:51:LYS:CE	2.66	0.44
1:A:377:THR:HB	1:A:378:PRO:CD	2.48	0.44
1:A:436:CYS:SG	1:A:447:CYS:C	3.01	0.44
1:A:447:CYS:O	1:A:451:HIS:HD2	2.01	0.44
1:A:448:SER:O	1:A:452:LEU:HB2	2.18	0.44
1:A:66:LEU:HD12	2:A:601:MLI:C3	2.48	0.43
1:A:119:PRO:HG2	1:A:174:LEU:HA	2.00	0.43
1:A:457:ASN:HA	1:A:483:ARG:NH1	2.33	0.43
1:A:465:LYS:HD2	1:A:466:THR:OG1	2.18	0.43
1:A:290:ALA:HA	3:A:607:SIN:H32	2.01	0.43
1:A:383:PRO:HB2	1:A:445:LEU:CD1	2.47	0.43
1:A:483:ARG:O	1:A:487:PHE:HD2	2.01	0.43
1:A:23:VAL:HB	1:A:43:VAL:HG23	1.99	0.43
1:A:147:TYR:O	1:A:148:PHE:C	2.60	0.43
1:A:114:LYS:CE	5:A:1038:HOH:O	2.65	0.43
1:A:34:CYS:O	1:A:139:TYR:OH	2.22	0.43
1:A:208:ARG:H	1:A:208:ARG:CD	2.31	0.43
1:A:462:LEU:CD2	1:A:465:LYS:HE3	2.48	0.43
1:A:473:THR:HA	5:A:904:HOH:O	2.18	0.43
1:A:28:SER:CB	1:A:142:ALA:HB3	2.48	0.43
1:A:73:LYS:HA	1:A:73:LYS:HD3	1.70	0.43
1:A:156:HIS:HE1	5:A:734:HOH:O	2.02	0.43
1:A:524:LYS:CE	1:A:551:SER:OG	2.66	0.43
1:A:242:LYS:HG2	1:A:246:HIS:CD2	2.54	0.43
1:A:465:LYS:HD2	1:A:466:THR:CB	2.48	0.43
1:A:414:ALA:N	1:A:415:PRO:CD	2.82	0.42
1:A:134:LEU:HA	1:A:134:LEU:HD23	1.79	0.42
1:A:149:TYR:CD2	1:A:152:GLU:CG	3.01	0.42
1:A:150:GLY:O	1:A:153:LEU:N	2.49	0.42
1:A:221:LYS:HA	1:A:294:GLU:HA	2.01	0.42
1:A:117:PRO:C	1:A:119:PRO:HD3	2.44	0.42
1:A:196:ARG:HD2	1:A:196:ARG:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LEU:HD23	1:A:90:CYS:SG	2.60	0.42
1:A:103:LEU:HD11	1:A:246:HIS:HA	2.01	0.42
1:A:218:LEU:HD13	1:A:233:ILE:CG2	2.48	0.42
1:A:262:TYR:O	1:A:266:HIS:CD2	2.66	0.42
1:A:528:LEU:HD22	1:A:547:LEU:HD22	2.00	0.42
1:A:462:LEU:O	1:A:465:LYS:CD	2.67	0.42
1:A:220:GLN:NE2	1:A:340:TYR:O	2.51	0.42
1:A:274:LEU:HD22	1:A:289:ILE:HG12	2.02	0.42
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.84	0.42
1:A:315:CYS:SG	1:A:365:PRO:CB	3.08	0.42
1:A:409:ARG:HG2	1:A:413:LYS:CE	2.45	0.42
1:A:484:ARG:HB3	1:A:485:PRO:CD	2.49	0.42
1:A:445:LEU:N	1:A:446:PRO:HD2	2.34	0.42
1:A:207:GLU:HG3	1:A:238:THR:HG21	2.01	0.42
1:A:3:HIS:HA	5:A:1034:HOH:O	2.19	0.42
1:A:28:SER:HB2	1:A:142:ALA:CB	2.50	0.42
1:A:191:SER:HB2	5:A:854:HOH:O	2.20	0.42
1:A:213:TRP:HB3	5:A:747:HOH:O	2.20	0.42
1:A:274:LEU:O	1:A:275:LYS:C	2.63	0.42
1:A:419:THR:OG1	1:A:530:GLU:OE2	2.37	0.42
3:A:607:SIN:H31	5:A:871:HOH:O	2.20	0.42
1:A:218:LEU:CD1	1:A:233:ILE:HG22	2.50	0.41
1:A:383:PRO:O	1:A:387:VAL:HG23	2.20	0.41
1:A:528:LEU:HA	1:A:531:LEU:HD12	2.02	0.41
1:A:337:HIS:C	1:A:339:ASP:N	2.74	0.41
1:A:406:LEU:HD13	1:A:429:LEU:HB2	2.02	0.41
1:A:27:PHE:CG	1:A:74:LEU:HD21	2.55	0.41
1:A:510:ALA:HA	1:A:567:PHE:CE2	2.54	0.41
1:A:93:LYS:O	1:A:98:ARG:HB2	2.21	0.41
1:A:428:THR:O	1:A:432:VAL:HG23	2.20	0.41
1:A:429:LEU:HD21	1:A:455:ALA:HB3	2.02	0.41
1:A:20:LYS:HD2	1:A:47:THR:HG21	2.02	0.41
1:A:87:LEU:HD23	1:A:87:LEU:HA	1.65	0.41
1:A:184:LEU:O	1:A:188:ILE:HG12	2.21	0.41
1:A:118:GLU:HG2	5:A:980:HOH:O	2.20	0.41
1:A:133:PHE:CZ	1:A:164:PHE:CE1	3.08	0.41
1:A:219:SER:O	1:A:335:ARG:HA	2.20	0.41
1:A:221:LYS:NZ	1:A:290:ALA:O	2.54	0.41
1:A:262:TYR:CE1	1:A:266:HIS:CD2	3.09	0.41
1:A:337:HIS:C	1:A:339:ASP:H	2.28	0.41
1:A:14:LEU:HD23	1:A:14:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97[B]:GLU:OE2	5:A:961:HOH:O	2.20	0.40
1:A:172:ASP:CG	1:A:175:ALA:HB3	2.45	0.40
1:A:560:ARG:CD	1:A:561:GLU:N	2.84	0.40
1:A:164:PHE:CE2	1:A:181:LEU:HD21	2.56	0.40
1:A:264:CYS:SG	1:A:285:LYS:HD3	2.61	0.40
1:A:373:PHE:HA	1:A:376:PHE:CE2	2.55	0.40
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.76	0.40
1:A:346:LEU:O	1:A:350:LYS:HG2	2.22	0.40
1:A:408:VAL:HA	1:A:532:VAL:HG21	2.04	0.40
1:A:458:ARG:O	1:A:462:LEU:HG	2.22	0.40
1:A:34:CYS:N	1:A:84:TYR:OH	2.54	0.40
1:A:67:HIS:NE2	1:A:248:ASP:OD1	2.53	0.40
1:A:126:PHE:HB2	1:A:133:PHE:CE2	2.57	0.40
1:A:205:PHE:O	5:A:746:HOH:O	2.22	0.40
4:A:608:LMR:C1	5:A:736:HOH:O	2.68	0.40
1:A:502:LYS:HA	1:A:502:LYS:HD3	1.94	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	590/583 (101%)	567 (96%)	22 (4%)	1 (0%)	43 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	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	517/508 (102%)	498 (96%)	19 (4%)	30	25

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	HIS
1	A	34	CYS
1	A	67	HIS
1	A	73	LYS
1	A	120	ASP
1	A	161	LYS
1	A	208	ARG
1	A	244	CYS
1	A	370	ARG
1	A	397	VAL
1	A	425	ILE
1	A	434	SER
1	A	452	LEU
1	A	474	LYS
1	A	491	GLU
1	A	493	ASP
1	A	561	GLU
1	A	580	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	12	ASN
1	A	94	GLN
1	A	127	GLN
1	A	204	ASN
1	A	246	HIS

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Mol	Chain	Res	Type
1	A	266	HIS
1	A	267	GLN
1	A	284	GLN
1	A	317	HIS
1	A	457	ASN

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](#)

8 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$
3	SIN	A	607	-	7,7,7	0.99	0	8,8,8	1.86	3 (37%)
4	LMR	A	608	-	8,8,8	1.66	1 (12%)	10,10,10	2.42	5 (50%)
2	MLI	A	601	-	6,6,6	1.00	0	7,7,7	1.44	1 (14%)
2	MLI	A	606	-	6,6,6	1.15	0	7,7,7	1.14	0
2	MLI	A	605	-	6,6,6	1.14	0	7,7,7	1.70	1 (14%)
2	MLI	A	604	-	6,6,6	1.15	0	7,7,7	1.49	2 (28%)
2	MLI	A	603	-	6,6,6	1.29	1 (16%)	7,7,7	0.84	0
2	MLI	A	602	-	6,6,6	1.41	1 (16%)	7,7,7	1.28	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
3	SIN	A	607	-	-	2/5/5/5	-
4	LMR	A	608	-	-	4/8/8/8	-
2	MLI	A	601	-	-	0/4/4/4	-
2	MLI	A	606	-	-	0/4/4/4	-
2	MLI	A	605	-	-	0/4/4/4	-
2	MLI	A	604	-	-	0/4/4/4	-
2	MLI	A	603	-	-	2/4/4/4	-
2	MLI	A	602	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	LMR	C2-C1	-3.03	1.48	1.52
2	A	602	MLI	O9-C3	-2.23	1.23	1.30
2	A	603	MLI	O9-C3	-2.02	1.24	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	608	LMR	O2-C2-C3	4.85	121.63	109.96
4	A	608	LMR	O1A-C1-C2	-3.56	115.50	122.60
4	A	608	LMR	C3-C2-C1	-3.18	102.73	110.53
3	A	607	SIN	O2-C1-C2	3.02	123.53	114.00
2	A	605	MLI	C3-C1-C2	-3.00	102.36	112.95
2	A	601	MLI	O6-C2-C1	-2.44	115.16	122.11
3	A	607	SIN	O2-C1-O1	-2.31	117.40	123.33
4	A	608	LMR	O1B-C1-O1A	2.28	129.25	124.08
2	A	604	MLI	O9-C3-C1	2.23	121.41	114.51
3	A	607	SIN	O4-C4-C3	2.22	121.03	114.00
2	A	604	MLI	O7-C2-C1	2.12	121.07	114.51
4	A	608	LMR	O2-C2-C1	-2.02	105.23	110.36

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	608	LMR	O1A-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	608	LMR	O1B-C1-C2-O2
4	A	608	LMR	O2-C2-C3-C4
4	A	608	LMR	C1-C2-C3-C4
3	A	607	SIN	C1-C2-C3-C4
2	A	602	MLI	C3-C1-C2-O6
2	A	603	MLI	C3-C1-C2-O7
2	A	603	MLI	C3-C1-C2-O6
2	A	602	MLI	C3-C1-C2-O7
2	A	602	MLI	C2-C1-C3-O9
2	A	602	MLI	C2-C1-C3-O8
3	A	607	SIN	C2-C3-C4-O4

There are no ring outliers.

6 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	607	SIN	6	0
4	A	608	LMR	13	0
2	A	601	MLI	10	0
2	A	606	MLI	5	0
2	A	604	MLI	1	0
2	A	603	MLI	5	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	583/583 (100%)	0.32	25 (4%)	40 40	20, 40, 64, 91	9 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	LEU	5.0
1	A	2	THR	4.2
1	A	370	ARG	3.6
1	A	78	ALA	3.3
1	A	70	PHE	3.3
1	A	3	HIS	3.2
1	A	84	TYR	3.1
1	A	85	GLY	2.8
1	A	59	ALA	2.5
1	A	80	LEU	2.4
1	A	318	TYR	2.3
1	A	37[A]	GLU	2.2
1	A	178	ILE	2.2
1	A	164	PHE	2.2
1	A	116	LYS	2.2
1	A	175	ALA	2.2
1	A	306	ALA	2.1
1	A	170	ALA	2.1
1	A	293[A]	LYS	2.1
1	A	81	ARG	2.1
1	A	583	ALA	2.1
1	A	560	ARG	2.0
1	A	83	THR	2.0
1	A	82	ALA	2.0
1	A	67	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MLI	A	602	7/7	0.75	0.13	55,56,58,59	0
2	MLI	A	601	7/7	0.78	0.15	49,53,56,57	0
4	LMR	A	608	9/9	0.78	0.15	50,51,55,61	0
2	MLI	A	605	7/7	0.83	0.13	43,44,55,56	0
2	MLI	A	606	7/7	0.85	0.14	50,52,54,55	0
2	MLI	A	603	7/7	0.85	0.14	63,66,68,69	0
2	MLI	A	604	7/7	0.89	0.19	68,71,72,74	0
3	SIN	A	607	8/8	0.90	0.12	37,39,42,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.