



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:32 PM UTC

PDB ID : 2ZQZ / pdb_00002zqz
Title : R-state structure of allosteric L-lactate dehydrogenase from *Lactobacillus casei*
Authors : Arai, K.; Ishimitsu, T.; Fushinobu, S.; Uchikoba, H.; Matsuzawa, H.; Taguchi, H.
Deposited on : 2008-08-22
Resolution : 2.50 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:

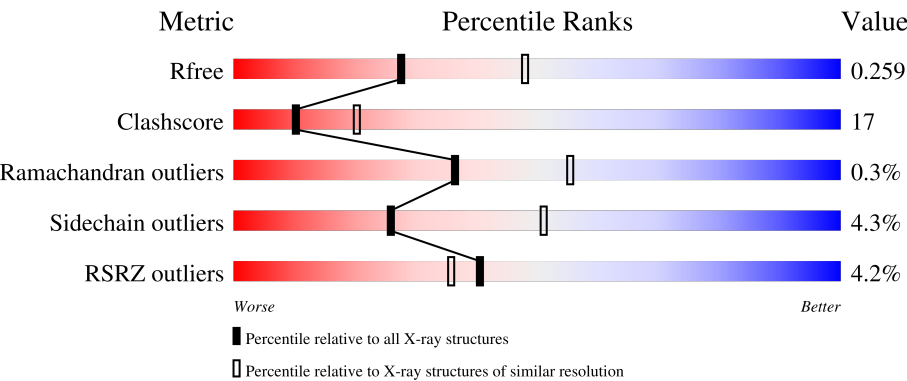
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	326	4% 63% 28% • 6%
1	B	326	2% 68% 24% • •
1	C	326	3% 60% 28% • 9%
1	D	326	8% 60% 30% • 6%
1	E	326	4% 65% 26% 5% •

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Mol	Chain	Length	Quality of chain
1	F	326	3% 68% 25% • •

2 Entry composition [i](#)

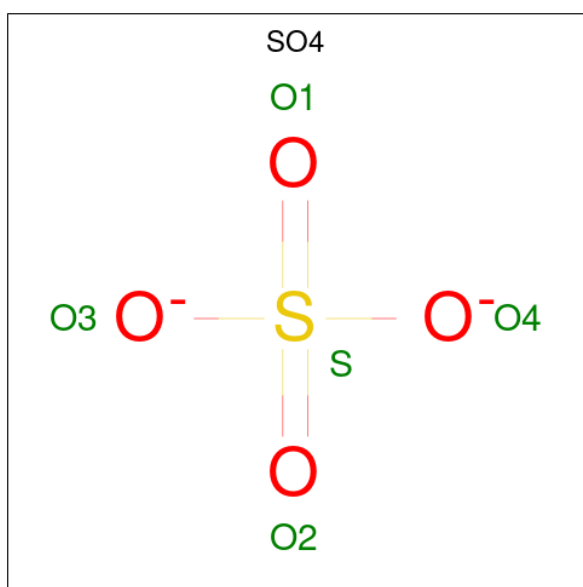
There are 3 unique types of molecules in this entry. The entry contains 14550 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2356	1505	391	454	6			
1	B	313	Total	C	N	O	S	0	0	0
			2399	1531	399	463	6			
1	C	297	Total	C	N	O	S	0	0	0
			2282	1457	378	441	6			
1	D	307	Total	C	N	O	S	0	0	0
			2356	1505	391	454	6			
1	E	312	Total	C	N	O	S	0	0	0
			2394	1528	398	462	6			
1	F	313	Total	C	N	O	S	0	0	0
			2399	1531	399	463	6			

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



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

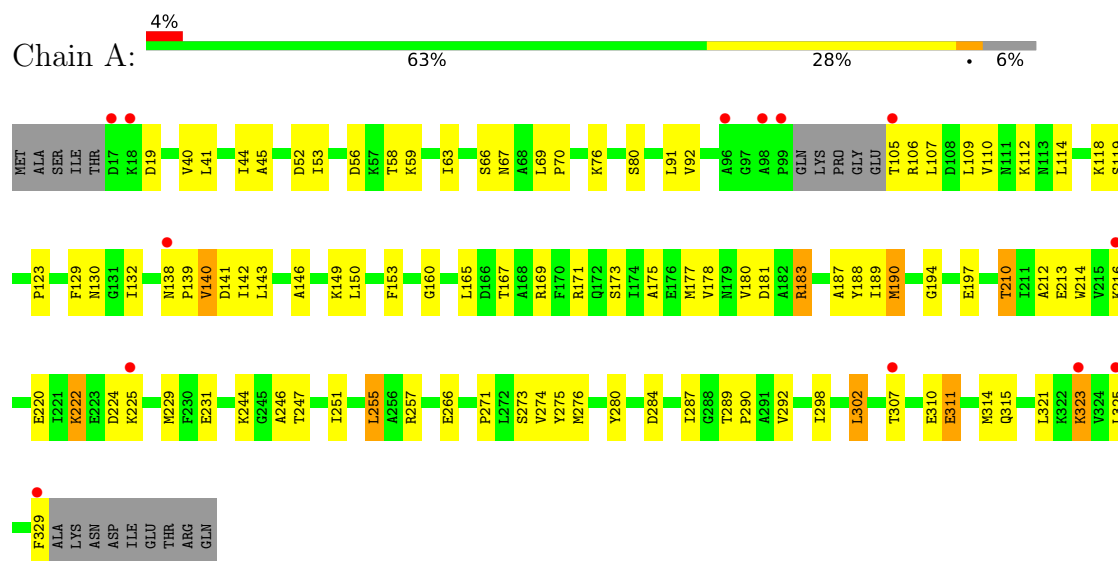
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	51	Total O 51 51	0	0
3	B	62	Total O 62 62	0	0
3	C	46	Total O 46 46	0	0
3	D	46	Total O 46 46	0	0
3	E	53	Total O 53 53	0	0
3	F	46	Total O 46 46	0	0

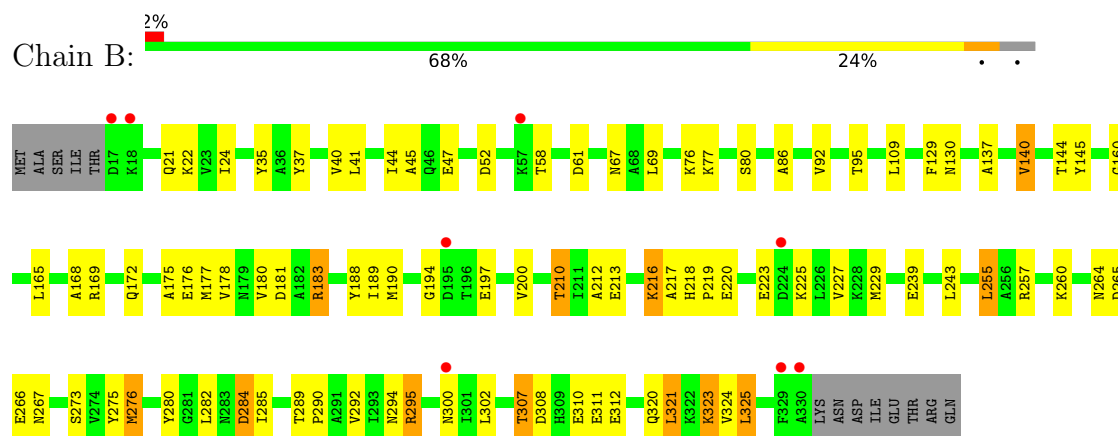
3 Residue-property plots

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

• Molecule 1: L-lactate dehydrogenase

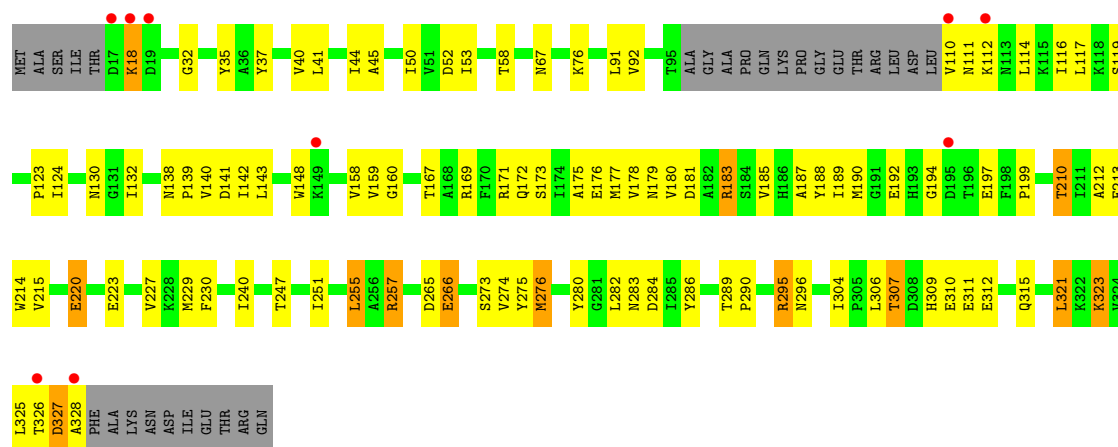


• Molecule 1: L-lactate dehydrogenase

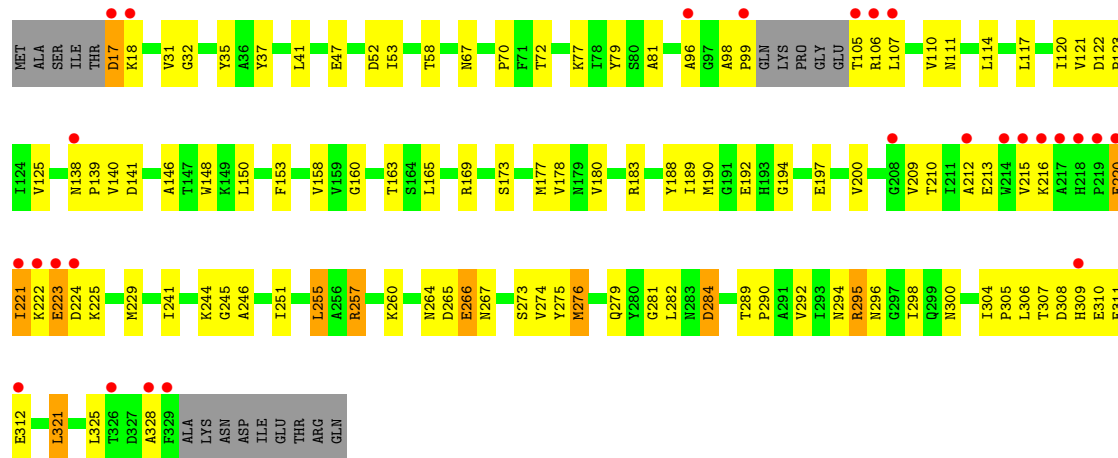


• Molecule 1: L-lactate dehydrogenase

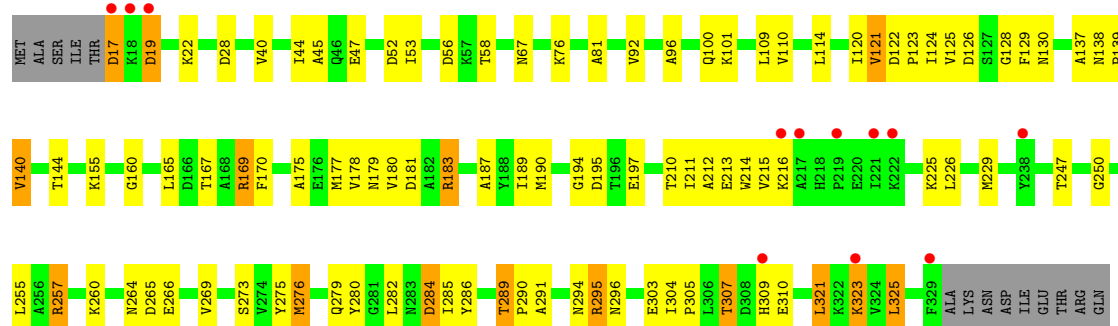




• Molecule 1: L-lactate dehydrogenase

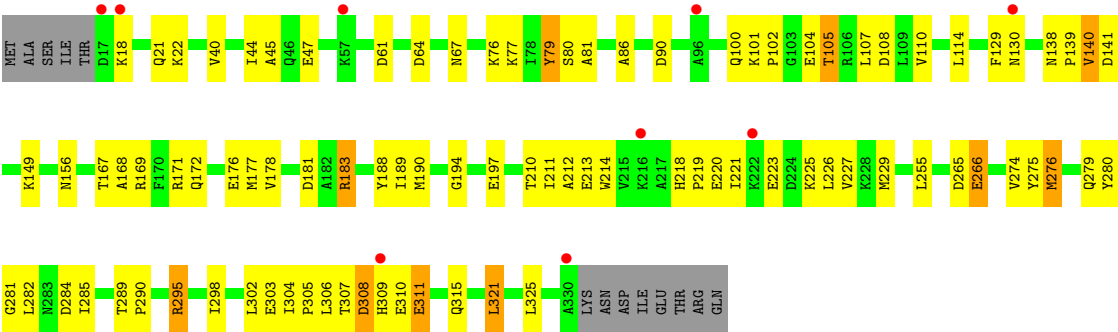


• Molecule 1: L-lactate dehydrogenase



• Molecule 1: L-lactate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.38Å 82.89Å 179.77Å 90.00° 91.21° 90.00°	Depositor
Resolution (Å)	34.10 – 2.50 34.10 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (34.10-2.50) 99.9 (34.10-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.271 0.215 , 0.259	Depositor DCC
R_{free} test set	9142 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14550	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: 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	0.41	0/2398	0.93	5/3252 (0.2%)
1	B	0.41	0/2443	0.97	10/3314 (0.3%)
1	C	0.42	0/2322	0.91	4/3148 (0.1%)
1	D	0.40	0/2398	0.91	5/3252 (0.2%)
1	E	0.43	0/2438	0.94	6/3307 (0.2%)
1	F	0.41	0/2443	0.94	6/3314 (0.2%)
All	All	0.41	0/14442	0.94	36/19587 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	VAL	N-CA-C	8.71	118.78	110.42
1	C	18	LYS	N-CA-C	8.45	123.14	110.64
1	F	140	VAL	N-CA-C	8.20	118.26	110.30
1	D	223	GLU	N-CA-C	-8.19	102.39	112.38
1	A	189	ILE	N-CA-C	-8.12	96.74	108.11
1	B	189	ILE	N-CA-C	-7.42	97.73	108.11
1	E	140	VAL	N-CA-C	7.27	117.40	110.42
1	E	189	ILE	N-CA-C	-7.05	98.25	108.11
1	A	140	VAL	N-CA-C	7.00	117.51	110.23
1	F	189	ILE	N-CA-C	-6.98	98.07	108.12
1	D	220	GLU	N-CA-C	-6.96	103.69	111.28
1	A	266	GLU	N-CA-C	6.67	121.16	112.89
1	F	308	ASP	N-CA-C	-6.67	103.94	111.07
1	F	266	GLU	N-CA-C	6.40	120.83	112.89
1	E	144	THR	N-CA-C	-6.36	104.43	111.36
1	C	189	ILE	N-CA-C	-6.35	98.31	107.78
1	B	284	ASP	N-CA-C	6.22	120.20	112.24
1	B	95	THR	N-CA-C	6.21	123.40	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	ILE	N-CA-C	-6.12	98.82	107.75
1	B	144	THR	N-CA-C	-6.08	104.28	111.03
1	B	95	THR	CA-C-N	-6.01	113.51	123.37
1	B	95	THR	C-N-CA	-6.01	113.51	123.37
1	E	284	ASP	N-CA-C	6.01	119.68	111.39
1	E	121	VAL	N-CA-C	5.82	116.47	110.36
1	B	109	LEU	N-CA-C	-5.57	105.29	111.36
1	C	266	GLU	N-CA-C	5.56	120.13	113.23
1	C	307	THR	N-CA-C	-5.52	103.09	110.55
1	A	190	MET	N-CA-C	5.37	117.56	109.41
1	D	266	GLU	N-CA-C	5.32	119.82	113.23
1	D	284	ASP	N-CA-C	5.24	118.67	111.54
1	E	81	ALA	N-CA-C	5.22	117.79	109.65
1	F	80	SER	N-CA-C	-5.15	101.36	109.25
1	B	80	SER	N-CA-C	-5.08	102.34	109.96
1	A	80	SER	N-CA-C	-5.04	102.39	109.96
1	F	79	TYR	N-CA-C	5.01	116.46	108.79
1	B	69	LEU	N-CA-C	5.01	119.76	113.25

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	2356	0	2374	74	0
1	B	2399	0	2417	74	0
1	C	2282	0	2299	96	0
1	D	2356	0	2374	111	0
1	E	2394	0	2412	82	0
1	F	2399	0	2417	80	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	10	0	0	0	0
3	A	51	0	0	5	0
3	B	62	0	0	2	0
3	C	46	0	0	2	0
3	D	46	0	0	5	0
3	E	53	0	0	2	0
3	F	46	0	0	3	0
All	All	14550	0	14293	487	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 17.

All (487) 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:276:MET:HG2	1:D:282:LEU:HB2	1.32	1.07
1:C:276:MET:HG2	1:C:282:LEU:HB2	1.34	1.03
1:B:276:MET:HG2	1:B:282:LEU:HB2	1.42	0.99
1:E:210:THR:HG22	1:E:212:ALA:H	1.26	0.99
1:D:210:THR:HG22	1:D:212:ALA:H	1.33	0.94
1:B:307:THR:HG22	1:B:310:GLU:H	1.30	0.92
1:F:210:THR:HB	1:F:213:GLU:HG3	1.53	0.89
1:D:222:LYS:HB2	1:D:225:LYS:HG3	1.56	0.88
1:E:307:THR:HG22	1:E:310:GLU:H	1.39	0.88
1:E:276:MET:HG2	1:E:282:LEU:HB2	1.56	0.87
1:F:276:MET:HG2	1:F:282:LEU:HB2	1.59	0.83
1:F:265:ASP:OD1	1:F:295:ARG:HB3	1.78	0.83
1:D:210:THR:HB	1:D:213:GLU:HG3	1.63	0.81
1:C:192:GLU:OE2	1:C:321:LEU:HD23	1.81	0.81
1:E:210:THR:HB	1:E:213:GLU:HG3	1.62	0.80
1:D:274:VAL:HG13	1:D:298:ILE:HD13	1.64	0.80
1:A:169:ARG:HD3	1:B:67:ASN:OD1	1.82	0.80
1:E:212:ALA:O	1:E:216:LYS:HD3	1.83	0.78
1:C:210:THR:HG22	1:C:213:GLU:H	1.48	0.78
1:D:105:THR:HG22	1:D:107:LEU:H	1.46	0.77
1:E:177:MET:HE2	1:E:225:LYS:HD3	1.66	0.77
1:D:177:MET:HE3	1:D:229:MET:HE3	1.67	0.76
1:A:40:VAL:HA	1:A:76:LYS:HE2	1.68	0.75
1:C:290:PRO:HG2	1:C:304:ILE:HD11	1.68	0.75
1:D:212:ALA:O	1:D:215:VAL:HG12	1.85	0.75
1:D:216:LYS:H	1:D:216:LYS:HD2	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:HD12	1:B:41:LEU:HD12	1.70	0.74
1:E:210:THR:HG22	1:E:212:ALA:N	2.03	0.73
1:A:311:GLU:O	1:A:315:GLN:HG2	1.89	0.72
1:D:213:GLU:CD	1:E:305:PRO:HG3	2.13	0.72
1:D:122:ASP:HB2	1:D:123:PRO:HD3	1.71	0.72
1:E:276:MET:HE3	1:E:276:MET:HA	1.70	0.72
1:B:40:VAL:HA	1:B:76:LYS:HE2	1.72	0.71
1:B:323:LYS:NZ	1:B:323:LYS:HB3	2.06	0.71
1:B:210:THR:HG22	1:B:213:GLU:H	1.56	0.70
1:C:172:GLN:O	1:C:176:GLU:HG3	1.93	0.69
1:B:210:THR:HB	1:B:213:GLU:HG3	1.73	0.69
1:D:178:VAL:HG12	1:D:180:VAL:HG23	1.74	0.68
1:F:274:VAL:HG12	1:F:298:ILE:HD13	1.76	0.68
1:C:212:ALA:O	1:C:215:VAL:HG12	1.93	0.67
1:C:295:ARG:HD2	1:D:18:LYS:HB3	1.75	0.67
1:D:194:GLY:O	1:D:197:GLU:HG2	1.95	0.67
1:F:177:MET:HE3	1:F:229:MET:HE3	1.76	0.67
1:E:190:MET:HE3	1:E:289:THR:HG23	1.75	0.67
1:A:210:THR:HB	1:A:213:GLU:HG3	1.77	0.67
1:C:223:GLU:O	1:C:227:VAL:HG23	1.93	0.67
1:C:67:ASN:OD1	1:E:169:ARG:HD3	1.95	0.66
1:C:296:ASN:HD21	1:D:18:LYS:HE3	1.59	0.66
1:F:190:MET:HE3	1:F:289:THR:HA	1.78	0.66
1:A:251:ILE:HG13	1:A:255:LEU:HD22	1.78	0.66
1:F:177:MET:HE3	1:F:229:MET:CE	2.26	0.65
1:B:194:GLY:O	1:B:197:GLU:HG2	1.96	0.65
1:C:169:ARG:HH22	1:C:240:ILE:HD12	1.61	0.65
1:A:105:THR:HG22	1:A:107:LEU:H	1.62	0.65
1:E:307:THR:HG21	3:E:348:HOH:O	1.95	0.65
1:A:194:GLY:O	1:A:197:GLU:HG2	1.96	0.65
1:B:276:MET:HE3	1:B:276:MET:HA	1.77	0.65
1:E:211:ILE:O	1:E:215:VAL:HG23	1.97	0.65
1:E:323:LYS:NZ	1:E:323:LYS:HB3	2.11	0.65
1:F:105:THR:HG22	1:F:108:ASP:H	1.62	0.64
1:C:214:TRP:HZ3	1:F:302:LEU:HD11	1.62	0.64
1:F:177:MET:HE1	1:F:226:LEU:HD23	1.79	0.64
1:D:190:MET:HE3	1:D:289:THR:HG23	1.79	0.64
1:D:220:GLU:CD	1:D:220:GLU:H	2.06	0.64
1:C:265:ASP:OD1	1:C:295:ARG:HB3	1.99	0.63
1:D:244:LYS:HE2	1:D:246:ALA:O	1.98	0.63
1:C:276:MET:HE3	1:C:276:MET:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:TYR:CZ	1:F:284:ASP:HA	2.32	0.63
1:C:18:LYS:HB3	1:D:295:ARG:HD2	1.79	0.63
1:E:289:THR:HG22	1:E:290:PRO:HD2	1.80	0.62
1:F:306:LEU:HB3	1:F:310:GLU:HB2	1.80	0.62
1:D:67:ASN:OD1	1:F:169:ARG:HD3	2.00	0.62
1:C:18:LYS:HE2	1:D:296:ASN:HD21	1.64	0.61
1:D:138:ASN:HA	1:D:140:VAL:N	2.15	0.61
1:D:222:LYS:HB2	1:D:225:LYS:CG	2.29	0.61
1:E:276:MET:HE2	1:E:279:GLN:HB2	1.82	0.61
1:B:308:ASP:O	1:B:312:GLU:HG3	2.00	0.61
1:D:307:THR:HB	1:D:310:GLU:HG3	1.81	0.61
1:C:194:GLY:O	1:C:197:GLU:HG2	2.01	0.60
1:D:120:ILE:O	1:D:123:PRO:HD2	2.01	0.60
1:D:307:THR:HG22	1:D:308:ASP:N	2.15	0.60
1:F:110:VAL:O	1:F:114:LEU:HG	2.02	0.60
1:F:307:THR:HG22	1:F:309:HIS:H	1.66	0.60
1:B:289:THR:HG22	1:B:290:PRO:HD2	1.83	0.60
1:F:40:VAL:HA	1:F:76:LYS:HE2	1.83	0.60
1:A:160:GLY:HA3	1:A:273:SER:OG	2.01	0.60
1:C:173:SER:OG	1:C:229:MET:HG3	2.01	0.60
1:D:215:VAL:HG13	1:D:216:LYS:HD2	1.83	0.59
1:C:40:VAL:HA	1:C:76:LYS:HE2	1.84	0.59
1:C:190:MET:HE3	1:C:289:THR:HA	1.85	0.59
1:D:192:GLU:OE2	1:D:321:LEU:HD23	2.02	0.59
1:D:275:TYR:CZ	1:D:284:ASP:HA	2.37	0.59
1:C:178:VAL:HG12	1:C:180:VAL:HG23	1.85	0.59
1:F:307:THR:HG22	1:F:308:ASP:N	2.16	0.59
1:F:177:MET:HE2	1:F:225:LYS:HD3	1.84	0.59
1:E:178:VAL:HG12	1:E:180:VAL:HG23	1.84	0.59
1:F:210:THR:HG22	1:F:212:ALA:H	1.68	0.59
1:D:138:ASN:HD22	1:D:140:VAL:H	1.50	0.59
1:F:290:PRO:HG2	1:F:304:ILE:HD11	1.85	0.59
1:B:178:VAL:HG12	1:B:178:VAL:O	2.03	0.59
1:B:86:ALA:O	1:B:129:PHE:HB2	2.02	0.58
1:B:190:MET:HE1	1:B:280:TYR:CZ	2.37	0.58
1:C:307:THR:CG2	1:C:310:GLU:H	2.15	0.58
1:D:305:PRO:HG3	1:E:213:GLU:CD	2.27	0.58
1:E:92:VAL:HG11	1:E:124:ILE:HD13	1.85	0.58
1:B:275:TYR:CZ	1:B:284:ASP:HA	2.38	0.58
1:D:117:LEU:O	1:D:121:VAL:HG23	2.04	0.58
1:B:177:MET:HE3	1:B:229:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:ASP:OD2	1:F:183:ARG:HD3	2.03	0.58
1:B:172:GLN:O	1:B:176:GLU:HG3	2.04	0.58
1:C:240:ILE:CG2	1:C:247:THR:HG22	2.33	0.58
1:D:210:THR:HG22	1:D:212:ALA:N	2.12	0.58
1:F:275:TYR:OH	1:F:284:ASP:HA	2.03	0.58
1:B:47:GLU:HG3	1:B:77:LYS:HB3	1.86	0.58
1:C:167:THR:HG23	1:C:187:ALA:O	2.03	0.57
1:C:296:ASN:HD21	1:D:18:LYS:CE	2.17	0.57
1:D:106:ARG:HH21	1:D:106:ARG:HG2	1.69	0.57
1:E:265:ASP:OD1	1:E:294:ASN:HB2	2.05	0.57
1:E:296:ASN:HD21	1:F:18:LYS:HE2	1.70	0.57
1:F:274:VAL:HG12	1:F:298:ILE:CD1	2.34	0.57
1:C:181:ASP:OD2	1:C:183:ARG:HD3	2.05	0.57
1:D:70:PRO:HG2	1:F:168:ALA:HB1	1.86	0.56
1:D:307:THR:O	1:D:311:GLU:HB2	2.04	0.56
1:A:177:MET:HE3	1:A:229:MET:HE3	1.87	0.56
1:D:307:THR:HG22	1:D:309:HIS:H	1.71	0.56
1:B:276:MET:HA	1:B:276:MET:CE	2.36	0.56
1:F:105:THR:HG22	1:F:107:LEU:N	2.21	0.56
1:B:177:MET:HE2	1:B:225:LYS:HE3	1.88	0.56
1:C:306:LEU:HB3	1:C:310:GLU:HB2	1.87	0.56
1:E:137:ALA:O	1:E:140:VAL:HA	2.07	0.55
1:F:100:GLN:HA	1:F:104:GLU:OE1	2.07	0.55
1:D:215:VAL:HA	3:D:350:HOH:O	2.06	0.55
1:A:210:THR:HG22	1:A:213:GLU:H	1.71	0.55
1:D:215:VAL:HG21	1:D:223:GLU:OE1	2.05	0.55
1:E:178:VAL:HG12	1:E:178:VAL:O	2.06	0.55
1:F:178:VAL:HG12	1:F:178:VAL:O	2.07	0.55
1:A:275:TYR:OH	1:A:284:ASP:HA	2.07	0.55
1:E:175:ALA:HB1	1:E:180:VAL:O	2.07	0.55
1:C:210:THR:HG23	3:C:366:HOH:O	2.07	0.55
1:C:323:LYS:NZ	1:C:323:LYS:HB3	2.21	0.55
1:A:210:THR:HG23	3:A:369:HOH:O	2.05	0.55
1:C:169:ARG:HD3	1:E:67:ASN:OD1	2.06	0.55
1:E:155:LYS:HD3	1:E:275:TYR:CD2	2.42	0.54
1:B:265:ASP:OD1	1:B:295:ARG:HB3	2.07	0.54
1:F:188:TYR:CE2	1:F:290:PRO:HG3	2.42	0.54
1:A:119:SER:O	1:A:123:PRO:HG3	2.07	0.54
1:D:165:LEU:O	1:D:169:ARG:HG3	2.08	0.54
1:D:221:ILE:O	1:D:222:LYS:HG2	2.07	0.54
1:E:120:ILE:O	1:E:123:PRO:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:THR:HB	1:C:213:GLU:HG3	1.90	0.54
1:D:265:ASP:OD1	1:D:294:ASN:HB2	2.07	0.54
1:D:138:ASN:HA	1:D:140:VAL:H	1.70	0.54
1:F:194:GLY:O	1:F:197:GLU:HG2	2.08	0.54
1:F:220:GLU:H	1:F:220:GLU:CD	2.16	0.54
1:A:178:VAL:HG12	1:A:178:VAL:O	2.08	0.54
1:F:79:TYR:CE2	1:F:81:ALA:HB2	2.42	0.53
1:A:167:THR:O	1:A:171:ARG:HG3	2.07	0.53
1:A:275:TYR:CZ	1:A:284:ASP:HA	2.44	0.53
1:B:175:ALA:HB1	1:B:180:VAL:O	2.09	0.53
1:F:149:LYS:HG3	3:F:367:HOH:O	2.08	0.53
1:C:110:VAL:HG12	1:C:114:LEU:HD12	1.89	0.53
1:D:17:ASP:OD2	1:D:17:ASP:N	2.40	0.53
1:A:210:THR:HB	1:A:213:GLU:CG	2.39	0.53
1:C:307:THR:HG22	1:C:310:GLU:H	1.74	0.52
1:A:173:SER:OG	1:A:229:MET:HG3	2.10	0.52
1:F:190:MET:HE1	1:F:280:TYR:CZ	2.44	0.52
1:C:130:ASN:CG	1:C:130:ASN:O	2.51	0.52
1:E:100:GLN:HB3	1:E:109:LEU:HD13	1.91	0.52
1:F:221:ILE:HD12	1:F:221:ILE:N	2.24	0.52
1:B:285:ILE:HD12	1:B:321:LEU:HD12	1.91	0.52
1:D:274:VAL:CG1	1:D:298:ILE:HD13	2.37	0.52
1:C:321:LEU:O	1:C:325:LEU:HB2	2.10	0.52
1:E:269:VAL:HA	1:E:291:ALA:O	2.09	0.52
1:C:117:LEU:HD22	1:C:143:LEU:HD22	1.92	0.52
1:E:260:LYS:O	1:E:264:ASN:HB2	2.10	0.52
1:C:169:ARG:NH2	1:C:240:ILE:HD12	2.25	0.52
1:D:307:THR:CG2	1:D:308:ASP:N	2.73	0.52
1:E:138:ASN:HA	1:E:140:VAL:N	2.25	0.52
1:E:121:VAL:O	1:E:125:VAL:HG23	2.10	0.52
1:B:92:VAL:HG23	1:B:129:PHE:CZ	2.46	0.51
1:D:47:GLU:HG3	1:D:77:LYS:HB3	1.93	0.51
1:E:40:VAL:HA	1:E:76:LYS:HE2	1.92	0.51
1:B:210:THR:HG22	1:B:212:ALA:N	2.26	0.51
1:A:175:ALA:HB1	1:A:180:VAL:O	2.10	0.51
1:B:22:LYS:HE3	1:B:47:GLU:OE2	2.10	0.51
1:C:257:ARG:NH1	1:C:266:GLU:OE1	2.43	0.51
1:F:190:MET:HE1	1:F:280:TYR:OH	2.11	0.51
1:B:178:VAL:HG12	1:B:180:VAL:HG23	1.93	0.51
1:B:290:PRO:O	1:B:302:LEU:HB2	2.11	0.51
1:E:323:LYS:HB3	1:E:323:LYS:HZ2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:321:LEU:HD22	1:F:321:LEU:O	2.11	0.51
1:A:67:ASN:OD1	1:B:169:ARG:HD3	2.10	0.51
1:B:188:TYR:CE2	1:B:290:PRO:HG3	2.45	0.51
1:D:148:TRP:HA	1:D:158:VAL:HG21	1.92	0.51
1:E:177:MET:HE3	1:E:229:MET:CE	2.41	0.51
1:F:311:GLU:O	1:F:315:GLN:HG2	2.11	0.51
1:A:109:LEU:HA	1:A:112:LYS:HE2	1.91	0.51
1:A:287:ILE:HD13	1:A:314:MET:HE3	1.92	0.51
1:E:19:ASP:H	1:F:295:ARG:HG3	1.76	0.51
1:C:188:TYR:CE2	1:C:290:PRO:HG3	2.45	0.50
1:D:274:VAL:HG13	1:D:298:ILE:CD1	2.37	0.50
1:F:172:GLN:O	1:F:176:GLU:HG3	2.11	0.50
1:B:177:MET:HE3	1:B:229:MET:HE3	1.93	0.50
1:C:295:ARG:HD2	1:D:18:LYS:HE2	1.94	0.50
1:D:289:THR:HG22	1:D:290:PRO:HD2	1.94	0.50
1:B:216:LYS:HD2	1:B:216:LYS:N	2.26	0.50
1:B:260:LYS:HG3	1:B:264:ASN:ND2	2.25	0.50
1:A:130:ASN:HA	1:A:153:PHE:CZ	2.47	0.50
1:C:276:MET:HA	1:C:276:MET:CE	2.41	0.50
1:F:167:THR:O	1:F:171:ARG:HG3	2.12	0.50
1:B:218:HIS:N	1:B:219:PRO:HD3	2.26	0.50
1:D:290:PRO:HG2	1:D:304:ILE:HD11	1.92	0.50
1:D:216:LYS:H	1:D:216:LYS:CD	2.21	0.50
1:E:285:ILE:HD12	1:E:321:LEU:HD12	1.93	0.50
1:A:53:ILE:HG13	3:A:383:HOH:O	2.12	0.50
1:B:177:MET:CE	1:B:225:LYS:HE3	2.42	0.50
1:F:130:ASN:CG	1:F:130:ASN:O	2.54	0.50
1:A:210:THR:HB	1:A:213:GLU:CD	2.37	0.50
1:B:61:ASP:CG	3:B:347:HOH:O	2.55	0.49
1:C:190:MET:HE1	1:C:280:TYR:CZ	2.47	0.49
1:C:311:GLU:O	1:C:315:GLN:HG2	2.12	0.49
1:A:178:VAL:HG11	1:A:214:TRP:CZ2	2.47	0.49
1:A:210:THR:HG22	1:A:212:ALA:N	2.27	0.49
1:A:190:MET:HE1	1:A:280:TYR:CZ	2.46	0.49
1:B:44:ILE:O	1:B:45:ALA:HB3	2.13	0.49
1:D:188:TYR:CE2	1:D:290:PRO:HG3	2.47	0.49
1:F:140:VAL:HG13	1:F:141:ASP:N	2.27	0.49
1:F:218:HIS:N	1:F:219:PRO:HD3	2.28	0.49
1:C:327:ASP:O	1:C:328:ALA:HB2	2.13	0.49
1:D:79:TYR:CE2	1:D:81:ALA:HB2	2.48	0.49
1:B:137:ALA:O	1:B:140:VAL:HA	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:THR:CG2	1:C:213:GLU:HG3	2.42	0.49
1:E:280:TYR:HE2	1:E:289:THR:HG21	1.77	0.49
1:E:160:GLY:HA3	1:E:273:SER:OG	2.12	0.49
1:E:177:MET:HE3	1:E:229:MET:HE3	1.95	0.49
1:F:138:ASN:CG	1:F:139:PRO:HA	2.38	0.49
1:A:212:ALA:O	1:A:216:LYS:HD3	2.13	0.49
1:B:177:MET:HE2	1:B:225:LYS:CD	2.42	0.49
1:A:110:VAL:O	1:A:114:LEU:HG	2.12	0.49
1:F:47:GLU:HG3	1:F:77:LYS:HB3	1.94	0.49
1:C:18:LYS:HD3	1:D:295:ARG:HH11	1.78	0.48
1:D:146:ALA:O	1:D:150:LEU:HG	2.13	0.48
1:E:276:MET:HA	1:E:276:MET:CE	2.42	0.48
1:F:44:ILE:O	1:F:45:ALA:HB3	2.12	0.48
1:A:140:VAL:HG13	1:A:141:ASP:N	2.28	0.48
1:C:140:VAL:HG13	1:C:141:ASP:N	2.27	0.48
1:C:177:MET:HE3	1:C:229:MET:CE	2.43	0.48
1:E:165:LEU:HD13	1:E:250:GLY:C	2.39	0.48
1:A:222:LYS:HB3	1:A:224:ASP:OD1	2.12	0.48
1:B:165:LEU:O	1:B:169:ARG:HG3	2.13	0.48
1:C:111:ASN:N	1:C:111:ASN:OD1	2.43	0.48
1:D:275:TYR:CE2	1:D:284:ASP:HA	2.48	0.48
1:C:50:ILE:HG22	1:C:58:THR:HG22	1.95	0.48
1:C:177:MET:SD	1:C:229:MET:HE1	2.54	0.48
1:C:213:GLU:CD	1:F:305:PRO:HG3	2.38	0.48
1:C:295:ARG:HH11	1:D:18:LYS:HE2	1.77	0.48
1:C:307:THR:HG23	1:C:309:HIS:N	2.28	0.48
1:C:323:LYS:HB3	1:C:323:LYS:HZ3	1.78	0.48
1:C:177:MET:HE3	1:C:229:MET:HE1	1.95	0.48
1:C:251:ILE:HG13	1:C:255:LEU:HD22	1.96	0.48
1:E:52:ASP:HB3	1:E:58:THR:CG2	2.43	0.48
1:F:190:MET:CE	1:F:289:THR:HG23	2.44	0.48
1:A:307:THR:HG22	1:A:310:GLU:CG	2.44	0.47
1:C:307:THR:HG22	1:C:310:GLU:CG	2.44	0.47
1:F:190:MET:HE3	1:F:289:THR:HG23	1.96	0.47
1:B:223:GLU:O	1:B:227:VAL:HG23	2.14	0.47
1:D:200:VAL:HG12	1:D:200:VAL:O	2.13	0.47
1:D:265:ASP:CG	1:D:295:ARG:HE	2.21	0.47
1:E:100:GLN:HB3	1:E:109:LEU:HD22	1.95	0.47
1:F:21:GLN:HA	1:F:90:ASP:OD2	2.14	0.47
1:A:167:THR:HG23	1:A:187:ALA:O	2.15	0.47
1:C:240:ILE:HG21	1:C:247:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:THR:O	1:C:326:THR:HG22	2.14	0.47
1:E:257:ARG:NH1	1:E:266:GLU:OE1	2.46	0.47
1:D:70:PRO:CG	1:F:168:ALA:HB1	2.44	0.47
1:C:276:MET:CG	1:C:282:LEU:HB2	2.24	0.47
1:B:292:VAL:HB	1:B:300:ASN:H	1.79	0.47
1:D:110:VAL:O	1:D:114:LEU:HG	2.14	0.47
1:E:138:ASN:HD22	1:E:140:VAL:H	1.62	0.47
1:A:181:ASP:OD2	1:A:183:ARG:HD3	2.14	0.47
1:A:307:THR:CG2	1:A:310:GLU:H	2.28	0.47
1:B:289:THR:HG22	1:B:290:PRO:CD	2.44	0.47
1:B:289:THR:CG2	1:B:290:PRO:HD2	2.45	0.47
1:D:178:VAL:HG12	1:D:178:VAL:O	2.15	0.47
1:E:52:ASP:HB3	1:E:58:THR:HG21	1.97	0.47
1:A:149:LYS:HD3	1:A:329:PHE:CE2	2.49	0.47
1:B:280:TYR:HE2	1:B:289:THR:HG21	1.80	0.47
1:E:170:PHE:CE2	1:E:187:ALA:HB1	2.50	0.47
1:A:138:ASN:HA	1:A:140:VAL:N	2.30	0.47
1:C:44:ILE:O	1:C:45:ALA:HB3	2.15	0.47
1:D:210:THR:HB	1:D:213:GLU:CG	2.41	0.47
1:F:274:VAL:CG1	1:F:298:ILE:HD13	2.45	0.47
1:A:287:ILE:HD13	1:A:314:MET:CE	2.44	0.46
1:D:37:TYR:CZ	1:D:41:LEU:HD11	2.49	0.46
1:A:178:VAL:CG1	1:A:214:TRP:CZ2	2.98	0.46
1:C:307:THR:HG22	1:C:310:GLU:HG3	1.96	0.46
1:D:215:VAL:HG13	1:D:216:LYS:N	2.30	0.46
1:E:17:ASP:N	1:E:17:ASP:OD2	2.47	0.46
1:A:118:LYS:HA	1:A:150:LEU:HD13	1.97	0.46
1:A:106:ARG:HH22	1:A:142:ILE:HD11	1.79	0.46
1:A:274:VAL:HG12	1:A:298:ILE:CD1	2.46	0.46
1:F:285:ILE:HD12	1:F:321:LEU:HD12	1.98	0.46
1:D:41:LEU:HA	1:D:72:THR:HG21	1.98	0.46
1:E:178:VAL:HG13	1:E:214:TRP:CZ2	2.50	0.46
1:F:307:THR:CG2	1:F:308:ASP:N	2.78	0.46
1:A:289:THR:OG1	1:A:290:PRO:HD2	2.16	0.46
1:C:295:ARG:CD	1:D:18:LYS:HB3	2.44	0.46
1:F:289:THR:CG2	1:F:290:PRO:HD2	2.46	0.46
1:B:266:GLU:O	1:B:267:ASN:HB2	2.16	0.46
1:D:221:ILE:HG23	1:D:222:LYS:N	2.30	0.46
1:E:138:ASN:HA	1:E:139:PRO:C	2.41	0.46
1:E:178:VAL:O	1:E:178:VAL:CG1	2.64	0.46
1:B:160:GLY:HA3	1:B:273:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:MET:CE	1:B:225:LYS:HG2	2.46	0.45
1:A:323:LYS:NZ	1:A:323:LYS:HB3	2.32	0.45
1:B:320:GLN:O	1:B:324:VAL:HG23	2.16	0.45
1:D:173:SER:OG	1:D:229:MET:HG3	2.16	0.45
1:F:289:THR:HG22	1:F:290:PRO:N	2.32	0.45
1:D:274:VAL:HG22	1:D:298:ILE:HD13	1.99	0.45
1:D:307:THR:HG23	3:D:366:HOH:O	2.15	0.45
1:A:244:LYS:HE2	1:A:246:ALA:O	2.15	0.45
1:A:274:VAL:HG12	1:A:298:ILE:HD13	1.98	0.45
1:B:35:TYR:CD1	1:B:255:LEU:HB3	2.51	0.45
1:E:177:MET:HE2	1:E:225:LYS:CD	2.40	0.45
1:C:37:TYR:CZ	1:C:41:LEU:HD11	2.52	0.45
1:C:178:VAL:HG12	1:C:178:VAL:O	2.15	0.45
1:C:307:THR:HG23	1:C:309:HIS:H	1.80	0.45
1:E:126:ASP:C	1:E:128:GLY:H	2.24	0.45
1:F:156:ASN:HB2	1:F:298:ILE:O	2.16	0.45
1:D:213:GLU:OE2	1:E:305:PRO:HG3	2.17	0.45
1:E:295:ARG:HG2	1:E:296:ASN:N	2.31	0.45
1:D:122:ASP:CB	1:D:123:PRO:HD3	2.45	0.45
1:B:92:VAL:HG23	1:B:129:PHE:CE1	2.51	0.45
1:D:274:VAL:HG12	1:D:275:TYR:N	2.31	0.45
1:F:101:LYS:HB3	1:F:102:PRO:HD2	1.99	0.45
1:C:111:ASN:OD1	1:C:112:LYS:N	2.50	0.45
1:E:44:ILE:O	1:E:45:ALA:HB3	2.17	0.45
1:B:145:TYR:CD1	1:B:145:TYR:C	2.95	0.44
1:B:145:TYR:CD1	1:B:325:LEU:HD11	2.52	0.44
1:C:148:TRP:HA	1:C:158:VAL:HG21	1.99	0.44
1:F:279:GLN:HA	1:F:303:GLU:OE1	2.18	0.44
1:A:44:ILE:O	1:A:45:ALA:HB3	2.17	0.44
1:A:210:THR:CB	1:A:213:GLU:HG3	2.46	0.44
1:A:292:VAL:HG23	1:A:302:LEU:HD21	1.99	0.44
1:B:264:ASN:O	1:B:265:ASP:C	2.60	0.44
1:C:175:ALA:O	1:C:179:ASN:N	2.50	0.44
1:E:307:THR:HG23	1:E:309:HIS:H	1.81	0.44
1:F:178:VAL:HG11	1:F:214:TRP:CZ2	2.53	0.44
1:B:323:LYS:HB3	1:B:323:LYS:HZ2	1.78	0.44
1:D:140:VAL:HG13	1:D:141:ASP:N	2.31	0.44
1:E:181:ASP:OD2	1:E:183:ARG:HD3	2.17	0.44
1:E:289:THR:HG22	1:E:290:PRO:CD	2.47	0.44
1:A:178:VAL:HG12	1:A:180:VAL:HG23	2.00	0.44
1:B:178:VAL:O	1:B:178:VAL:CG1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ASP:HB3	1:D:58:THR:CG2	2.48	0.44
1:E:130:ASN:O	1:E:130:ASN:CG	2.61	0.44
1:D:177:MET:CE	1:D:229:MET:HE3	2.43	0.44
1:D:190:MET:CE	1:D:289:THR:HG23	2.45	0.44
1:B:323:LYS:HB3	1:B:323:LYS:HZ3	1.80	0.44
1:C:214:TRP:HZ3	1:F:302:LEU:CD1	2.31	0.44
1:A:70:PRO:HG3	1:B:168:ALA:HB1	2.00	0.44
1:C:92:VAL:HG11	1:C:124:ILE:HD13	1.98	0.44
1:C:276:MET:HE3	1:C:276:MET:CA	2.46	0.44
1:E:22:LYS:HE3	1:E:47:GLU:OE2	2.17	0.44
1:E:177:MET:HE1	1:E:226:LEU:HD23	1.98	0.44
1:E:325:LEU:HD12	1:E:325:LEU:HA	1.88	0.44
1:A:247:THR:HG23	3:A:343:HOH:O	2.18	0.43
1:C:171:ARG:HD3	1:C:185:VAL:O	2.18	0.43
1:C:199:PRO:HD3	1:C:230:PHE:CE1	2.53	0.43
1:B:220:GLU:CD	1:B:220:GLU:H	2.26	0.43
1:B:239:GLU:O	1:B:243:LEU:HG	2.18	0.43
1:C:119:SER:O	1:C:123:PRO:HG3	2.18	0.43
1:D:266:GLU:O	1:D:267:ASN:HB2	2.18	0.43
1:D:276:MET:HA	1:D:276:MET:HE2	2.00	0.43
1:E:122:ASP:HB2	1:E:123:PRO:HD3	1.99	0.43
1:E:275:TYR:CZ	1:E:284:ASP:HA	2.53	0.43
1:E:290:PRO:HG2	1:E:304:ILE:HD11	2.00	0.43
1:A:92:VAL:HG23	1:A:129:PHE:CZ	2.53	0.43
1:B:267:ASN:OD1	1:B:294:ASN:HB3	2.18	0.43
1:C:328:ALA:HB1	3:C:340:HOH:O	2.18	0.43
1:D:222:LYS:C	1:D:224:ASP:N	2.74	0.43
1:B:294:ASN:C	1:B:294:ASN:OD1	2.62	0.43
1:C:52:ASP:OD1	1:C:53:ILE:N	2.52	0.43
1:E:167:THR:HG23	1:E:187:ALA:O	2.19	0.43
1:A:91:LEU:HD12	1:A:132:ILE:O	2.18	0.43
1:D:114:LEU:HD11	1:D:328:ALA:HB1	2.00	0.43
1:C:160:GLY:HA3	1:C:273:SER:OG	2.19	0.43
1:C:274:VAL:O	1:C:286:TYR:HA	2.19	0.43
1:C:110:VAL:HG12	1:C:114:LEU:CD1	2.49	0.43
1:A:139:PRO:O	1:A:143:LEU:HG	2.19	0.43
1:E:52:ASP:OD1	1:E:53:ILE:N	2.52	0.43
1:F:210:THR:HG22	1:F:211:ILE:N	2.33	0.43
1:A:59:LYS:O	1:A:63:ILE:HG13	2.19	0.42
1:D:32:GLY:O	1:D:35:TYR:HB3	2.18	0.42
1:D:53:ILE:HG13	3:D:341:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:VAL:O	1:D:178:VAL:CG1	2.68	0.42
1:A:19:ASP:HA	3:A:357:HOH:O	2.18	0.42
1:A:56:ASP:O	1:B:243:LEU:HB3	2.19	0.42
1:B:24:ILE:HG13	1:B:86:ALA:HA	2.01	0.42
1:D:260:LYS:HG3	1:D:264:ASN:ND2	2.34	0.42
1:D:306:LEU:HB3	1:D:310:GLU:HB2	2.00	0.42
1:A:210:THR:CG2	1:A:213:GLU:HG3	2.48	0.42
1:C:276:MET:O	1:C:283:ASN:HA	2.19	0.42
1:D:289:THR:CG2	1:D:290:PRO:HD2	2.49	0.42
1:E:275:TYR:HD1	1:E:286:TYR:CE1	2.38	0.42
1:F:101:LYS:HE2	3:F:366:HOH:O	2.19	0.42
1:B:52:ASP:HB3	1:B:58:THR:CG2	2.50	0.42
1:C:295:ARG:HB3	1:C:295:ARG:HE	1.72	0.42
1:E:178:VAL:CG1	1:E:214:TRP:CZ2	3.02	0.42
1:F:86:ALA:O	1:F:129:PHE:HB2	2.20	0.42
1:F:177:MET:HE3	1:F:229:MET:HE1	2.00	0.42
1:A:187:ALA:HA	3:A:346:HOH:O	2.18	0.42
1:A:307:THR:HG22	1:A:310:GLU:HG3	2.02	0.42
1:D:31:VAL:HG13	1:D:251:ILE:HG23	2.00	0.42
1:D:107:LEU:HD11	1:D:328:ALA:HA	2.01	0.42
1:E:210:THR:HG22	1:E:211:ILE:N	2.34	0.42
1:D:35:TYR:CD1	1:D:255:LEU:HB3	2.54	0.42
1:C:190:MET:HE1	1:C:280:TYR:OH	2.20	0.42
1:F:210:THR:HG22	1:F:212:ALA:N	2.34	0.42
1:A:165:LEU:O	1:A:169:ARG:HG3	2.20	0.42
1:A:222:LYS:HB2	1:A:225:LYS:HG2	2.02	0.42
1:F:64:ASP:O	1:F:67:ASN:HB2	2.20	0.42
1:C:266:GLU:O	1:F:181:ASP:HB2	2.20	0.42
1:D:107:LEU:O	1:D:111:ASN:ND2	2.52	0.42
1:D:163:THR:HG23	3:D:360:HOH:O	2.19	0.42
1:E:110:VAL:O	1:E:114:LEU:HG	2.19	0.42
1:D:121:VAL:O	1:D:125:VAL:HG23	2.19	0.41
1:E:280:TYR:H	1:E:303:GLU:CD	2.28	0.41
1:B:276:MET:HE3	1:B:276:MET:CA	2.49	0.41
1:D:257:ARG:NH1	1:D:266:GLU:OE1	2.53	0.41
1:E:28:ASP:CG	1:E:28:ASP:O	2.62	0.41
1:E:194:GLY:O	1:E:197:GLU:HG2	2.20	0.41
1:F:275:TYR:C	1:F:275:TYR:CD2	2.98	0.41
1:B:130:ASN:O	1:B:130:ASN:CG	2.63	0.41
1:C:138:ASN:HA	1:C:139:PRO:C	2.44	0.41
1:C:312:GLU:O	1:C:315:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:ALA:O	1:E:179:ASN:N	2.53	0.41
1:E:92:VAL:HG23	1:E:129:PHE:CZ	2.55	0.41
1:C:159:VAL:HG12	1:C:160:GLY:N	2.35	0.41
1:C:220:GLU:CD	1:C:220:GLU:H	2.29	0.41
1:D:105:THR:HG22	1:D:107:LEU:N	2.24	0.41
1:D:160:GLY:HA3	1:D:273:SER:OG	2.21	0.41
1:D:279:GLN:C	1:D:281:GLY:H	2.28	0.41
1:F:105:THR:HG23	3:F:356:HOH:O	2.20	0.41
1:F:210:THR:HB	1:F:213:GLU:CG	2.39	0.41
1:F:289:THR:HG23	1:F:290:PRO:HD2	2.01	0.41
1:B:200:VAL:HB	3:B:350:HOH:O	2.20	0.41
1:D:241:ILE:HG23	1:D:245:GLY:O	2.21	0.41
1:F:223:GLU:O	1:F:227:VAL:HG23	2.20	0.41
1:A:52:ASP:HB3	1:A:58:THR:CG2	2.51	0.41
1:C:275:TYR:CZ	1:C:284:ASP:HA	2.55	0.41
1:D:148:TRP:CD1	1:D:153:PHE:O	2.74	0.41
1:F:22:LYS:HE3	1:F:47:GLU:OE2	2.21	0.41
1:A:139:PRO:HG2	1:A:142:ILE:HB	2.03	0.41
1:A:188:TYR:CE2	1:A:271:PRO:HG3	2.56	0.41
1:C:177:MET:CE	1:C:229:MET:HE1	2.51	0.41
1:D:292:VAL:HG21	1:D:300:ASN:HD22	1.85	0.41
1:D:308:ASP:O	1:D:312:GLU:HG3	2.21	0.41
1:F:279:GLN:C	1:F:281:GLY:H	2.29	0.41
1:A:66:SER:HA	1:A:69:LEU:HG	2.02	0.41
1:B:21:GLN:HB2	1:B:45:ALA:HA	2.03	0.41
1:D:106:ARG:HH21	1:D:106:ARG:CG	2.34	0.41
1:D:279:GLN:H	1:D:279:GLN:CD	2.29	0.41
1:E:165:LEU:O	1:E:169:ARG:HG3	2.20	0.41
1:E:247:THR:HG23	3:E:374:HOH:O	2.19	0.41
1:A:307:THR:HG23	1:A:310:GLU:H	1.85	0.40
1:C:91:LEU:HD12	1:C:132:ILE:O	2.21	0.40
1:C:116:ILE:O	1:C:119:SER:OG	2.35	0.40
1:D:98:ALA:HA	1:D:99:PRO:HD3	1.95	0.40
1:D:209:VAL:CG2	1:E:304:ILE:HD13	2.51	0.40
1:E:126:ASP:C	1:E:128:GLY:N	2.78	0.40
1:F:177:MET:HE1	1:F:226:LEU:CD2	2.48	0.40
1:B:181:ASP:OD1	1:B:183:ARG:HD3	2.21	0.40
1:D:255:LEU:HD12	1:D:255:LEU:HA	1.88	0.40
1:D:298:ILE:HD12	3:D:374:HOH:O	2.21	0.40
1:A:146:ALA:O	1:A:150:LEU:HG	2.21	0.40
1:A:276:MET:HA	1:A:276:MET:HE2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:HIS:HB3	1:F:220:GLU:OE2	2.22	0.40
1:A:105:THR:HG22	1:A:107:LEU:N	2.31	0.40
1:B:177:MET:HE3	1:B:229:MET:HE1	2.02	0.40
1:B:260:LYS:HG3	1:B:264:ASN:HD22	1.85	0.40
1:C:32:GLY:O	1:C:35:TYR:HB3	2.21	0.40
1:C:142:ILE:HG12	1:C:325:LEU:HD23	2.03	0.40
1:F:140:VAL:HG13	1:F:141:ASP:H	1.86	0.40
1:A:178:VAL:O	1:A:178:VAL:CG1	2.67	0.40
1:B:37:TYR:CE2	1:B:41:LEU:HD11	2.56	0.40
1:C:181:ASP:HB2	1:F:266:GLU:O	2.22	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	303/326 (93%)	288 (95%)	15 (5%)	0	100	100
1	B	311/326 (95%)	294 (94%)	16 (5%)	1 (0%)	36	55
1	C	293/326 (90%)	274 (94%)	18 (6%)	1 (0%)	36	55
1	D	303/326 (93%)	278 (92%)	22 (7%)	3 (1%)	12	24
1	E	310/326 (95%)	293 (94%)	16 (5%)	1 (0%)	36	55
1	F	311/326 (95%)	290 (93%)	21 (7%)	0	100	100
All	All	1831/1956 (94%)	1717 (94%)	108 (6%)	6 (0%)	36	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	327	ASP
1	B	217	ALA

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Mol	Chain	Res	Type
1	D	96	ALA
1	E	96	ALA
1	D	221	ILE
1	D	139	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	253/269 (94%)	241 (95%)	12 (5%)	23	47
1	B	257/269 (96%)	245 (95%)	12 (5%)	23	47
1	C	246/269 (91%)	237 (96%)	9 (4%)	30	57
1	D	253/269 (94%)	245 (97%)	8 (3%)	34	62
1	E	257/269 (96%)	241 (94%)	16 (6%)	16	34
1	F	257/269 (96%)	248 (96%)	9 (4%)	32	58
All	All	1523/1614 (94%)	1457 (96%)	66 (4%)	26	51

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	ARG
1	A	210	THR
1	A	220	GLU
1	A	222	LYS
1	A	231	GLU
1	A	255	LEU
1	A	257	ARG
1	A	302	LEU
1	A	311	GLU
1	A	321	LEU
1	A	323	LYS
1	A	325	LEU
1	B	183	ARG
1	B	210	THR

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Mol	Chain	Res	Type
1	B	216	LYS
1	B	255	LEU
1	B	257	ARG
1	B	276	MET
1	B	295	ARG
1	B	307	THR
1	B	311	GLU
1	B	321	LEU
1	B	323	LYS
1	B	325	LEU
1	C	183	ARG
1	C	210	THR
1	C	220	GLU
1	C	255	LEU
1	C	257	ARG
1	C	276	MET
1	C	295	ARG
1	C	321	LEU
1	C	323	LYS
1	D	17	ASP
1	D	183	ARG
1	D	255	LEU
1	D	257	ARG
1	D	276	MET
1	D	295	ARG
1	D	321	LEU
1	D	325	LEU
1	E	17	ASP
1	E	19	ASP
1	E	56	ASP
1	E	101	LYS
1	E	169	ARG
1	E	183	ARG
1	E	195	ASP
1	E	255	LEU
1	E	257	ARG
1	E	276	MET
1	E	289	THR
1	E	295	ARG
1	E	307	THR
1	E	321	LEU
1	E	323	LYS

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Mol	Chain	Res	Type
1	E	325	LEU
1	F	61	ASP
1	F	105	THR
1	F	183	ARG
1	F	255	LEU
1	F	276	MET
1	F	295	ARG
1	F	311	GLU
1	F	321	LEU
1	F	325	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	138	ASN
1	A	315	GLN
1	A	320	GLN
1	B	100	GLN
1	B	138	ASN
1	B	156	ASN
1	B	300	ASN
1	C	130	ASN
1	C	138	ASN
1	C	283	ASN
1	C	296	ASN
1	D	42	GLN
1	D	111	ASN
1	D	130	ASN
1	D	138	ASN
1	D	218	HIS
1	D	283	ASN
1	D	300	ASN
1	E	21	GLN
1	E	138	ASN
1	E	203	HIS
1	E	267	ASN
1	E	296	ASN
1	E	320	GLN
1	F	21	GLN
1	F	218	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	C	3	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	A	7	-	4,4,4	0.33	0	6,6,6	0.17	0
2	SO4	D	11	-	4,4,4	0.33	0	6,6,6	0.10	0
2	SO4	B	1	-	4,4,4	0.38	0	6,6,6	0.12	0
2	SO4	E	10	-	4,4,4	0.38	0	6,6,6	0.07	0
2	SO4	D	5	-	4,4,4	0.41	0	6,6,6	0.20	0
2	SO4	E	4	-	4,4,4	0.39	0	6,6,6	0.06	0
2	SO4	F	339	-	4,4,4	0.31	0	6,6,6	0.14	0
2	SO4	B	8	-	4,4,4	0.34	0	6,6,6	0.15	0
2	SO4	F	6	-	4,4,4	0.41	0	6,6,6	0.12	0
2	SO4	C	9	-	4,4,4	0.35	0	6,6,6	0.12	0
2	SO4	A	2	-	4,4,4	0.40	0	6,6,6	0.12	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	307/326 (94%)	0.09	13 (4%)	40 36	24, 40, 71, 88	0
1	B	313/326 (96%)	0.11	8 (2%)	57 52	23, 39, 63, 83	0
1	C	297/326 (91%)	0.07	9 (3%)	52 48	22, 39, 69, 89	0
1	D	307/326 (94%)	0.39	26 (8%)	16 14	25, 43, 90, 109	0
1	E	312/326 (95%)	-0.02	12 (3%)	44 39	23, 37, 66, 91	0
1	F	313/326 (96%)	0.10	9 (2%)	53 49	24, 40, 63, 91	0
All	All	1849/1956 (94%)	0.12	77 (4%)	40 36	22, 40, 71, 109	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	219	PRO	5.6
1	B	330	ALA	5.6
1	C	328	ALA	5.2
1	D	215	VAL	5.1
1	F	330	ALA	4.5
1	D	329	PHE	4.4
1	E	17	ASP	4.2
1	D	221	ILE	4.0
1	D	99	PRO	3.9
1	D	107	LEU	3.9
1	C	18	LYS	3.8
1	E	18	LYS	3.7
1	D	222	LYS	3.7
1	B	300	ASN	3.7
1	C	17	ASP	3.6
1	E	238	TYR	3.5
1	C	195	ASP	3.5
1	F	17	ASP	3.4
1	F	18	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	96	ALA	3.4
1	C	326	THR	3.3
1	D	18	LYS	3.3
1	A	225	LYS	3.2
1	D	216	LYS	3.2
1	A	17	ASP	3.1
1	D	309	HIS	3.1
1	D	105	THR	3.1
1	B	195	ASP	3.1
1	D	218	HIS	3.0
1	C	19	ASP	3.0
1	A	99	PRO	3.0
1	D	212	ALA	2.9
1	B	17	ASP	2.9
1	B	224	ASP	2.9
1	E	309	HIS	2.9
1	D	106	ARG	2.9
1	A	18	LYS	2.9
1	D	217	ALA	2.8
1	E	216	LYS	2.7
1	D	208	GLY	2.7
1	E	222	LYS	2.7
1	F	309	HIS	2.7
1	A	329	PHE	2.6
1	D	96	ALA	2.6
1	A	325	LEU	2.6
1	D	220	GLU	2.6
1	B	18	LYS	2.6
1	D	224	ASP	2.5
1	D	223	GLU	2.5
1	D	326	THR	2.5
1	C	149	LYS	2.4
1	F	216	LYS	2.4
1	F	222	LYS	2.4
1	E	221	ILE	2.4
1	D	17	ASP	2.3
1	F	57	LYS	2.3
1	D	214	TRP	2.2
1	E	219	PRO	2.2
1	A	307	THR	2.2
1	A	323	LYS	2.2
1	E	19	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	329	PHE	2.2
1	A	98	ALA	2.2
1	A	216	LYS	2.2
1	E	217	ALA	2.2
1	F	96	ALA	2.2
1	A	105	THR	2.2
1	E	329	PHE	2.2
1	C	110	VAL	2.1
1	C	112	LYS	2.1
1	A	138	ASN	2.1
1	D	328	ALA	2.1
1	D	138	ASN	2.1
1	F	130	ASN	2.1
1	D	312	GLU	2.1
1	B	57	LYS	2.1
1	E	323	LYS	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	SO4	D	5	5/5	0.93	0.09	43,44,60,68	0
2	SO4	F	6	5/5	0.95	0.07	43,46,61,62	0
2	SO4	B	1	5/5	0.96	0.07	38,47,55,61	0
2	SO4	A	2	5/5	0.97	0.05	42,48,56,59	0
2	SO4	E	4	5/5	0.97	0.05	36,37,52,54	0
2	SO4	E	10	5/5	0.97	0.06	39,46,49,54	0
2	SO4	C	3	5/5	0.97	0.06	50,52,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	8	5/5	0.98	0.04	34,39,43,43	0
2	SO4	F	339	5/5	0.98	0.05	33,35,39,41	0
2	SO4	A	7	5/5	0.99	0.05	33,35,43,44	0
2	SO4	D	11	5/5	0.99	0.05	33,37,39,45	0
2	SO4	C	9	5/5	0.99	0.05	31,36,41,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.