



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:08 PM UTC

PDB ID : 3DLK / pdb_00003dlk
Title : Crystal Structure of an engineered form of the HIV-1 Reverse Transcriptase, RT69A
Authors : Ho, W.C.; Bauman, J.D.; Himmel, D.M.; Das, K.; Arnold, E.
Deposited on : 2008-06-27
Resolution : 1.85 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

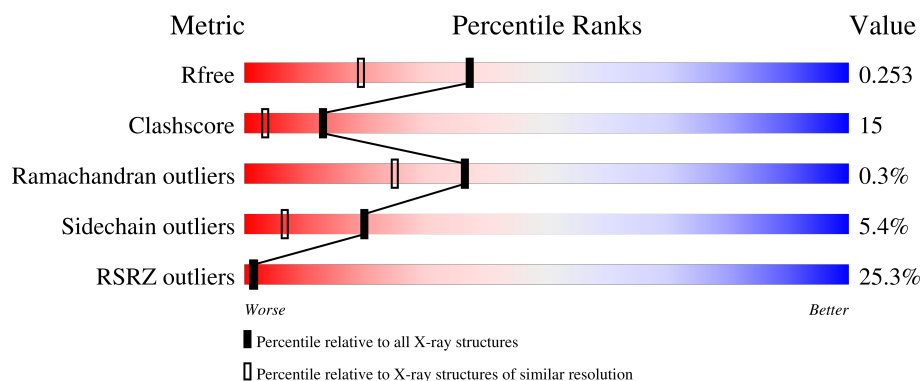
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	556	27% 71% 25% ..
2	B	423	22% 73% 19% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8069 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4489	2902	748	832	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P03366
A	160	SER	PHE	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	409	Total	C	N	O	S	0	0	0
			3388	2208	560	613	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

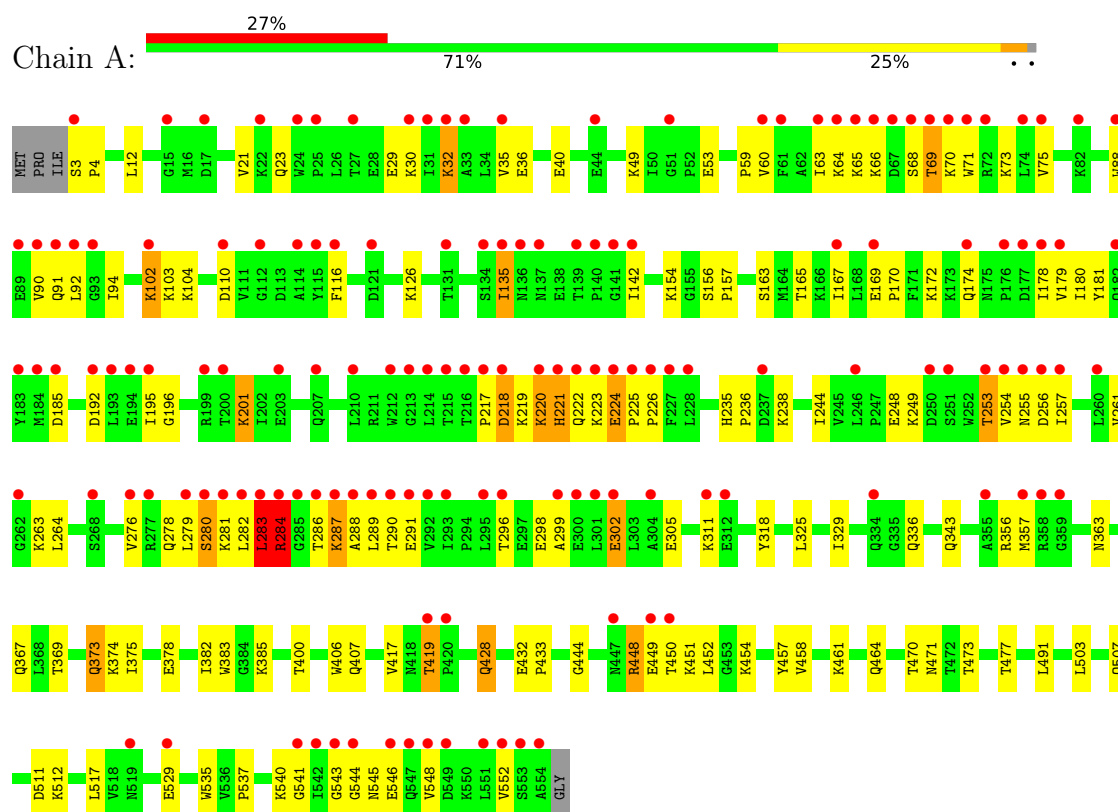
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total	O	0	0
			101	101		
4	B	86	Total	O	0	0
			86	86		

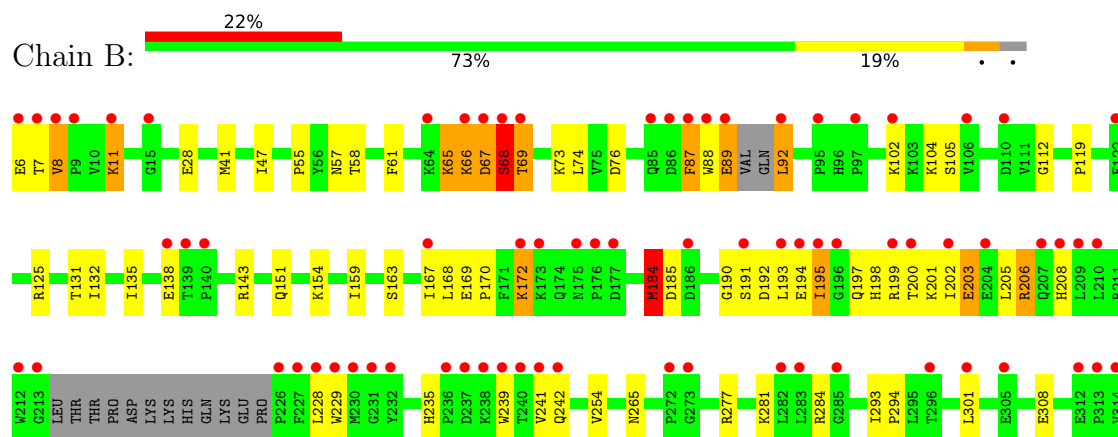
3 Residue-property plots [i](#)

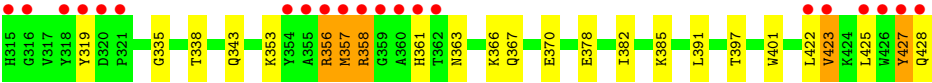
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Reverse transcriptase/ribonuclease H



• Molecule 2: p51 RT





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.01Å 72.04Å 109.33Å 90.00° 104.38° 90.00°	Depositor
Resolution (Å)	40.66 – 1.85 40.66 – 1.85	Depositor EDS
% Data completeness (in resolution range)	94.3 (40.66-1.85) 94.3 (40.66-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.250 0.237 , 0.253	Depositor DCC
R_{free} test set	2991 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8069	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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 [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	0.39	0/4605	0.93	13/6256 (0.2%)
2	B	0.41	1/3486 (0.0%)	0.91	13/4732 (0.3%)
All	All	0.40	1/8091 (0.0%)	0.92	26/10988 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	69	THR	CA-CB	5.30	1.60	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	THR	N-CA-C	9.49	124.32	110.28
2	B	401	TRP	N-CA-C	8.35	124.07	113.55
1	A	69	THR	N-CA-C	8.23	122.65	110.30
1	A	94	ILE	N-CA-C	8.12	115.96	107.76
1	A	249	LYS	N-CA-C	7.49	120.12	108.96
2	B	200	THR	N-CA-C	-7.16	102.89	111.69
1	A	281	LYS	N-CA-C	-7.10	102.96	113.61
2	B	87	PHE	N-CA-C	6.73	119.80	108.23
1	A	221	HIS	N-CA-C	-6.40	96.48	107.61
1	A	12	LEU	N-CA-C	-6.21	102.52	110.53
1	A	283	LEU	N-CA-C	5.97	117.90	110.91
2	B	68	SER	N-CA-C	5.96	118.69	110.35
1	A	284	ARG	N-CA-C	-5.85	104.28	112.12
2	B	69	THR	N-CA-C	-5.74	104.94	112.41
1	A	154	LYS	N-CA-C	5.67	118.19	111.33
2	B	343	GLN	N-CA-C	-5.65	106.31	113.43
2	B	132	ILE	N-CA-C	-5.63	102.07	107.76
1	A	382	ILE	N-CA-C	5.61	117.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	GLN	N-CA-C	-5.38	106.66	113.43
2	B	125	ARG	N-CA-C	5.30	117.74	111.33
2	B	382	ILE	N-CA-C	5.29	116.76	111.00
2	B	235	HIS	CA-C-N	5.25	124.69	119.24
2	B	235	HIS	C-N-CA	5.25	124.69	119.24
2	B	184	MET	CB-CA-C	-5.07	110.75	116.63
2	B	391	LEU	N-CA-C	5.05	116.03	109.72
1	A	220	LYS	N-CA-C	5.01	117.61	109.24

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	4489	0	4545	159	0
2	B	3388	0	3411	87	0
3	A	5	0	0	0	0
4	A	101	0	0	1	0
4	B	86	0	0	1	0
All	All	8069	0	7956	237	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 15.

All (237) 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:102:LYS:HE3	1:A:103:LYS:H	1.08	1.14
1:A:287:LYS:HB3	1:A:291:GLU:HG2	1.14	1.13
2:B:335:GLY:HA3	2:B:356:ARG:HG3	1.31	1.12
2:B:356:ARG:N	2:B:356:ARG:HD2	1.70	1.03
2:B:335:GLY:CA	2:B:356:ARG:HG3	1.91	1.00
2:B:41:MET:HE1	2:B:73:LYS:HE2	1.48	0.96
1:A:102:LYS:HE3	1:A:103:LYS:N	1.81	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:THR:HG22	2:B:143:ARG:HE	1.34	0.92
1:A:287:LYS:HB3	1:A:291:GLU:CG	2.01	0.89
1:A:287:LYS:CB	1:A:291:GLU:HG2	2.02	0.88
2:B:356:ARG:HD2	2:B:356:ARG:H	1.35	0.87
2:B:6:GLU:O	2:B:119:PRO:HG2	1.75	0.86
1:A:503:LEU:HD23	2:B:422:LEU:HD21	1.58	0.85
1:A:254:VAL:HG12	1:A:291:GLU:HB2	1.58	0.85
2:B:11:LYS:HE3	2:B:11:LYS:HA	1.60	0.82
1:A:284:ARG:HB3	1:A:284:ARG:CZ	2.08	0.81
1:A:284:ARG:HB3	1:A:284:ARG:NH1	1.94	0.81
2:B:356:ARG:N	2:B:356:ARG:CD	2.43	0.81
2:B:57:ASN:OD1	2:B:131:THR:HG23	1.80	0.80
1:A:444:GLY:HA2	1:A:552:VAL:HG11	1.64	0.79
2:B:357:MET:SD	2:B:358:ARG:HD3	2.22	0.78
2:B:335:GLY:C	2:B:356:ARG:HG3	2.08	0.78
1:A:288:ALA:O	1:A:289:LEU:HB3	1.85	0.77
1:A:369:THR:O	1:A:373:GLN:HG2	1.86	0.76
1:A:279:LEU:HG	1:A:302:GLU:OE2	1.86	0.75
2:B:281:LYS:HE2	2:B:284:ARG:NH2	2.01	0.75
2:B:356:ARG:HG2	2:B:358:ARG:O	1.88	0.74
1:A:223:LYS:HG2	1:A:224:GLU:H	1.53	0.74
1:A:278:GLN:HE21	1:A:298:GLU:CB	2.00	0.74
2:B:335:GLY:O	2:B:356:ARG:HG3	1.88	0.73
2:B:104:LYS:HG2	2:B:192:ASP:OD1	1.89	0.73
1:A:64:LYS:HA	1:A:70:LYS:O	1.88	0.72
1:A:278:GLN:HE21	1:A:298:GLU:HB3	1.53	0.71
1:A:503:LEU:CD2	2:B:422:LEU:HD21	2.19	0.71
2:B:172:LYS:HE2	2:B:172:LYS:HA	1.73	0.70
1:A:73:LYS:HZ3	1:A:75:VAL:HG23	1.57	0.70
2:B:335:GLY:HA3	2:B:356:ARG:CG	2.15	0.69
2:B:425:LEU:HD12	2:B:428:GLN:OE1	1.93	0.69
1:A:102:LYS:HA	1:A:102:LYS:CE	2.23	0.69
1:A:163:SER:O	1:A:167:ILE:HG12	1.94	0.67
1:A:255:ASN:HD22	1:A:288:ALA:HB1	1.60	0.67
2:B:338:THR:HG21	2:B:427:TYR:O	1.95	0.67
2:B:41:MET:HE3	2:B:47:ILE:HD13	1.75	0.66
2:B:366:LYS:O	2:B:370:GLU:HG3	1.95	0.66
2:B:335:GLY:O	2:B:356:ARG:CG	2.43	0.66
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.32	0.65
1:A:165:THR:O	1:A:169:GLU:HG3	1.97	0.64
1:A:325:LEU:HB2	1:A:385:LYS:HE3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLY:C	1:A:545:ASN:H	2.06	0.64
1:A:223:LYS:HG2	1:A:224:GLU:N	2.13	0.63
1:A:102:LYS:HD3	1:A:236:PRO:O	1.98	0.63
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.80	0.63
1:A:244:ILE:HD12	1:A:263:LYS:NZ	2.14	0.63
2:B:361:HIS:HD2	2:B:363:ASN:H	1.47	0.62
1:A:178:ILE:CD1	1:A:201:LYS:HG2	2.29	0.62
1:A:356:ARG:HD2	1:A:357:MET:O	1.99	0.62
1:A:3:SER:N	1:A:4:PRO:HD2	2.14	0.62
2:B:361:HIS:CD2	2:B:363:ASN:H	2.17	0.62
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.82	0.61
1:A:219:LYS:O	1:A:219:LYS:HG3	2.01	0.61
1:A:276:VAL:O	1:A:276:VAL:HG22	1.99	0.61
2:B:11:LYS:HA	2:B:11:LYS:CE	2.30	0.61
2:B:358:ARG:NH1	2:B:361:HIS:ND1	2.49	0.61
1:A:169:GLU:HB2	1:A:170:PRO:HD3	1.83	0.61
1:A:444:GLY:CA	1:A:552:VAL:HG11	2.30	0.61
1:A:64:LYS:HG2	1:A:70:LYS:C	2.26	0.60
2:B:254:VAL:HG22	2:B:293:ILE:HD11	1.83	0.60
1:A:400:THR:HG21	1:A:428:GLN:HE22	1.65	0.60
2:B:143:ARG:HD3	4:B:455:HOH:O	2.00	0.59
1:A:261:VAL:HG13	1:A:276:VAL:HG21	1.83	0.59
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.83	0.59
1:A:261:VAL:HG13	1:A:276:VAL:CG2	2.33	0.58
1:A:541:GLY:HA2	1:A:546:GLU:HG3	1.86	0.58
1:A:284:ARG:NH1	1:A:284:ARG:CB	2.66	0.58
1:A:491:LEU:HB3	1:A:529:GLU:HG2	1.85	0.58
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.85	0.57
1:A:253:THR:HA	1:A:291:GLU:O	2.03	0.57
1:A:511:ASP:O	1:A:512:LYS:HG3	2.05	0.57
1:A:543:GLY:C	1:A:545:ASN:N	2.61	0.57
2:B:169:GLU:N	2:B:170:PRO:HD2	2.18	0.57
2:B:281:LYS:HE2	2:B:284:ARG:CZ	2.35	0.57
2:B:356:ARG:O	2:B:356:ARG:HD3	2.05	0.57
1:A:64:LYS:HG3	1:A:71:TRP:CD2	2.40	0.56
2:B:168:LEU:HD22	2:B:205:LEU:HD11	1.86	0.56
1:A:135:ILE:HD13	1:A:135:ILE:H	1.70	0.56
2:B:67:ASP:OD1	2:B:68:SER:N	2.38	0.56
1:A:102:LYS:HD2	1:A:318:TYR:CD1	2.41	0.56
1:A:254:VAL:HG12	1:A:291:GLU:CB	2.34	0.55
1:A:282:LEU:O	1:A:283:LEU:HG	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:HD13	1:A:135:ILE:N	2.22	0.55
1:A:253:THR:HG22	1:A:256:ASP:OD2	2.07	0.55
1:A:64:LYS:HG2	1:A:70:LYS:O	2.07	0.55
1:A:102:LYS:HE3	1:A:102:LYS:HA	1.89	0.54
2:B:241:VAL:HG12	2:B:242:GLN:H	1.73	0.54
2:B:198:HIS:O	2:B:202:ILE:HG12	2.06	0.54
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.43	0.54
1:A:276:VAL:O	1:A:280:SER:HB2	2.07	0.54
1:A:543:GLY:H	1:A:546:GLU:HG2	1.71	0.54
1:A:167:ILE:O	1:A:170:PRO:HD2	2.07	0.54
1:A:223:LYS:HG2	1:A:224:GLU:HG3	1.88	0.54
1:A:279:LEU:N	1:A:302:GLU:OE2	2.40	0.54
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.08	0.54
1:A:287:LYS:CB	1:A:291:GLU:CG	2.76	0.53
1:A:461:LYS:HB3	1:A:461:LYS:NZ	2.24	0.53
1:A:255:ASN:HB2	1:A:288:ALA:HB1	1.89	0.53
1:A:552:VAL:HG12	1:A:552:VAL:O	2.08	0.53
2:B:335:GLY:O	2:B:356:ARG:HB3	2.10	0.52
1:A:540:LYS:HE3	2:B:265:ASN:OD1	2.09	0.52
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.90	0.52
1:A:296:THR:HG22	1:A:299:ALA:HB2	1.91	0.52
1:A:90:VAL:O	1:A:91:GLN:HB3	2.09	0.52
1:A:135:ILE:H	1:A:135:ILE:CD1	2.23	0.52
1:A:218:ASP:C	1:A:220:LYS:N	2.67	0.52
2:B:87:PHE:O	2:B:88:TRP:CD1	2.62	0.52
2:B:41:MET:CE	2:B:73:LYS:HE2	2.31	0.51
1:A:400:THR:HG21	1:A:428:GLN:NE2	2.25	0.51
1:A:110:ASP:OD1	1:A:217:PRO:HG2	2.10	0.51
1:A:223:LYS:CG	1:A:224:GLU:H	2.22	0.51
1:A:244:ILE:CG2	1:A:263:LYS:HZ1	2.23	0.51
1:A:543:GLY:O	1:A:545:ASN:N	2.36	0.51
1:A:104:LYS:HB3	1:A:192:ASP:HA	1.93	0.51
1:A:172:LYS:HE2	1:A:180:ILE:HB	1.93	0.50
1:A:110:ASP:HA	1:A:185:ASP:O	2.11	0.50
1:A:373:GLN:HE22	2:B:397:THR:HG23	1.76	0.50
2:B:112:GLY:HA3	2:B:151:GLN:HE21	1.77	0.50
1:A:450:THR:O	1:A:451:LYS:HB2	2.11	0.50
1:A:451:LYS:HB3	1:A:471:ASN:HA	1.93	0.50
2:B:241:VAL:HG12	2:B:242:GLN:N	2.26	0.50
2:B:8:VAL:HG11	2:B:159:ILE:HG23	1.94	0.50
1:A:544:GLY:O	1:A:548:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:THR:HG23	2:B:76:ASP:O	2.12	0.49
1:A:244:ILE:HG21	1:A:263:LYS:HZ1	1.77	0.49
1:A:181:TYR:CE2	2:B:138:GLU:HB3	2.48	0.49
2:B:191:SER:HG	2:B:198:HIS:HD1	1.60	0.49
1:A:218:ASP:C	1:A:220:LYS:H	2.20	0.49
2:B:88:TRP:O	2:B:89:GLU:HG3	2.12	0.49
1:A:278:GLN:HE21	1:A:298:GLU:HB2	1.75	0.49
1:A:296:THR:HG22	1:A:299:ALA:CB	2.43	0.48
1:A:458:VAL:HG12	1:A:464:GLN:HG2	1.95	0.48
1:A:244:ILE:HD12	1:A:263:LYS:HZ1	1.78	0.48
1:A:503:LEU:O	1:A:507:GLN:HG3	2.13	0.48
1:A:102:LYS:CD	1:A:318:TYR:CD1	2.96	0.48
1:A:36:GLU:O	1:A:40:GLU:HG3	2.14	0.48
2:B:88:TRP:C	2:B:89:GLU:HG3	2.38	0.48
1:A:66:LYS:C	1:A:68:SER:H	2.22	0.48
2:B:163:SER:O	2:B:167:ILE:HG13	2.13	0.48
2:B:6:GLU:HG2	2:B:7:THR:HG23	1.95	0.47
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.49	0.47
1:A:3:SER:N	1:A:4:PRO:CD	2.77	0.47
1:A:224:GLU:HB2	1:A:225:PRO:HD2	1.96	0.47
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.48	0.47
1:A:457:TYR:CD1	1:A:457:TYR:C	2.92	0.47
1:A:181:TYR:CD2	2:B:138:GLU:HB3	2.49	0.47
1:A:356:ARG:HG3	1:A:367:GLN:NE2	2.30	0.47
2:B:112:GLY:C	2:B:151:GLN:HE21	2.22	0.47
2:B:254:VAL:HG22	2:B:293:ILE:CD1	2.45	0.47
1:A:253:THR:CG2	1:A:256:ASP:OD2	2.62	0.47
2:B:105:SER:O	2:B:190:GLY:HA2	2.14	0.47
1:A:235:HIS:HB2	1:A:238:LYS:O	2.14	0.47
2:B:11:LYS:HE3	2:B:11:LYS:CA	2.38	0.47
2:B:193:LEU:CD1	2:B:201:LYS:HG3	2.44	0.47
2:B:194:GLU:H	2:B:197:GLN:HE21	1.63	0.47
2:B:335:GLY:O	2:B:356:ARG:CB	2.62	0.47
1:A:546:GLU:OE1	1:A:546:GLU:HA	2.14	0.46
1:A:253:THR:HG23	1:A:256:ASP:H	1.80	0.46
2:B:242:GLN:HE21	2:B:353:LYS:HB2	1.80	0.46
1:A:356:ARG:HG3	1:A:367:GLN:CD	2.41	0.46
1:A:473:THR:O	1:A:477:THR:HG23	2.16	0.46
1:A:53:GLU:N	1:A:53:GLU:OE1	2.49	0.45
2:B:358:ARG:HB3	2:B:361:HIS:HB2	1.99	0.45
1:A:179:VAL:CG2	1:A:181:TYR:CZ	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LYS:O	1:A:378:GLU:HG3	2.17	0.45
1:A:276:VAL:O	1:A:276:VAL:CG2	2.65	0.45
1:A:363:ASN:OD1	1:A:363:ASN:C	2.59	0.45
1:A:29:GLU:HG3	1:A:30:LYS:N	2.31	0.45
1:A:373:GLN:NE2	2:B:397:THR:OG1	2.50	0.45
2:B:69:THR:HG22	2:B:69:THR:O	2.17	0.45
1:A:102:LYS:CD	1:A:236:PRO:O	2.65	0.45
2:B:335:GLY:HA2	2:B:367:GLN:OE1	2.18	0.44
1:A:63:ILE:O	1:A:63:ILE:HG13	2.17	0.44
1:A:419:THR:O	1:A:419:THR:OG1	2.34	0.44
2:B:92:LEU:N	2:B:92:LEU:HD23	2.32	0.44
1:A:49:LYS:HE3	1:A:142:ILE:HG23	1.98	0.44
1:A:110:ASP:OD1	1:A:217:PRO:HD2	2.18	0.44
1:A:373:GLN:NE2	2:B:397:THR:HA	2.33	0.44
1:A:179:VAL:HG22	1:A:181:TYR:CE2	2.53	0.44
1:A:512:LYS:HD2	4:A:640:HOH:O	2.16	0.44
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.76	0.43
1:A:179:VAL:O	1:A:179:VAL:HG13	2.18	0.43
1:A:432:GLU:HB3	1:A:433:PRO:HD2	2.00	0.43
1:A:195:ILE:HG23	1:A:196:GLY:N	2.32	0.43
1:A:253:THR:O	1:A:257:ILE:HG13	2.18	0.43
1:A:503:LEU:HD22	1:A:535:TRP:HB2	2.00	0.43
1:A:102:LYS:HE3	1:A:102:LYS:CA	2.48	0.43
1:A:63:ILE:HA	1:A:71:TRP:HZ3	1.83	0.43
1:A:64:LYS:HG3	1:A:71:TRP:CE2	2.53	0.43
2:B:67:ASP:OD1	2:B:229:TRP:HH2	2.02	0.43
1:A:254:VAL:O	1:A:254:VAL:HG22	2.18	0.43
1:A:537:PRO:HB2	1:A:540:LYS:HG3	2.01	0.42
2:B:308:GLU:OE1	2:B:308:GLU:HA	2.19	0.42
2:B:67:ASP:CG	2:B:68:SER:N	2.76	0.42
2:B:228:LEU:HD23	2:B:228:LEU:O	2.18	0.42
1:A:102:LYS:CE	1:A:103:LYS:H	2.01	0.42
1:A:282:LEU:O	1:A:283:LEU:CG	2.67	0.42
1:A:283:LEU:CG	1:A:283:LEU:O	2.67	0.42
1:A:254:VAL:CG1	1:A:287:LYS:O	2.67	0.42
1:A:311:LYS:HA	1:A:311:LYS:HD2	1.82	0.42
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.50	0.42
2:B:195:ILE:HG12	2:B:199:ARG:CD	2.49	0.42
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.20	0.42
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.20	0.42
1:A:284:ARG:CB	1:A:284:ARG:HH11	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:VAL:O	1:A:417:VAL:HG13	2.19	0.41
2:B:65:LYS:O	2:B:66:LYS:C	2.63	0.41
1:A:65:LYS:HB2	1:A:68:SER:O	2.20	0.41
1:A:174:GLN:HE21	1:A:174:GLN:HB2	1.65	0.41
1:A:218:ASP:O	1:A:220:LYS:N	2.53	0.41
1:A:102:LYS:HD3	1:A:318:TYR:CE1	2.56	0.41
1:A:449:GLU:N	1:A:449:GLU:OE1	2.53	0.41
2:B:239:TRP:CH2	2:B:378:GLU:HA	2.55	0.41
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.51	0.41
2:B:112:GLY:CA	2:B:151:GLN:HE21	2.33	0.41
1:A:363:ASN:HA	1:A:511:ASP:CG	2.46	0.41
1:A:406:TRP:CE2	1:A:407:GLN:HG3	2.56	0.41
2:B:293:ILE:HA	2:B:294:PRO:HD3	1.95	0.41
1:A:135:ILE:N	1:A:135:ILE:CD1	2.83	0.41
1:A:417:VAL:HG22	1:A:419:THR:HG22	2.03	0.41
1:A:69:THR:O	1:A:70:LYS:CG	2.70	0.40
1:A:73:LYS:HZ3	1:A:75:VAL:CG2	2.28	0.40
2:B:203:GLU:HA	2:B:206:ARG:HB2	2.03	0.40
1:A:454:LYS:HB2	1:A:552:VAL:HG13	2.03	0.40
2:B:154:LYS:CA	2:B:184:MET:HE1	2.52	0.40
1:A:32:LYS:O	1:A:35:VAL:HG12	2.21	0.40
1:A:178:ILE:HD11	1:A:201:LYS:HG2	2.01	0.40
1:A:448:ARG:HG2	1:A:449:GLU:OE1	2.21	0.40
2:B:67:ASP:OD1	2:B:229:TRP:CH2	2.74	0.40
2:B:242:GLN:NE2	2:B:353:LYS:HB2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/556 (99%)	517 (94%)	32 (6%)	1 (0%)	43	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	403/423 (95%)	385 (96%)	16 (4%)	2 (0%)	24	13
All	All	953/979 (97%)	902 (95%)	48 (5%)	3 (0%)	36	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
2	B	66	LYS
2	B	423	VAL

5.3.2 Protein sidechains [i](#)

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	493/496 (99%)	468 (95%)	25 (5%)	21	7
2	B	371/385 (96%)	349 (94%)	22 (6%)	18	5
All	All	864/881 (98%)	817 (95%)	47 (5%)	20	7

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	102	LYS
1	A	116	PHE
1	A	126	LYS
1	A	135	ILE
1	A	201	LYS
1	A	218	ASP
1	A	221	HIS
1	A	224	GLU
1	A	248	GLU
1	A	253	THR
1	A	264	LEU
1	A	280	SER

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Mol	Chain	Res	Type
1	A	283	LEU
1	A	284	ARG
1	A	287	LYS
1	A	290	THR
1	A	302	GLU
1	A	305	GLU
1	A	336	GLN
1	A	373	GLN
1	A	419	THR
1	A	428	GLN
1	A	448	ARG
1	A	517	LEU
2	B	8	VAL
2	B	11	LYS
2	B	55	PRO
2	B	65	LYS
2	B	67	ASP
2	B	68	SER
2	B	89	GLU
2	B	92	LEU
2	B	102	LYS
2	B	172	LYS
2	B	184	MET
2	B	195	ILE
2	B	203	GLU
2	B	206	ARG
2	B	208	HIS
2	B	277	ARG
2	B	301	LEU
2	B	356	ARG
2	B	357	MET
2	B	358	ARG
2	B	423	VAL
2	B	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	161	GLN
1	A	174	GLN
1	A	182	GLN

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Mol	Chain	Res	Type
1	A	235	HIS
1	A	258	GLN
1	A	278	GLN
1	A	373	GLN
1	A	394	GLN
1	A	428	GLN
1	A	475	GLN
1	A	509	GLN
1	A	524	GLN
2	B	151	GLN
2	B	182	GLN
2	B	235	HIS
2	B	242	GLN
2	B	255	ASN
2	B	278	GLN
2	B	330	GLN
2	B	340	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](#)

1 ligand is 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	SO4	A	556	-	4,4,4	0.40	0	6,6,6	0.07	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 [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	552/556 (99%)	1.29	149 (26%)  	22, 47, 98, 146	0
2	B	409/423 (96%)	1.19	94 (22%)  	23, 43, 82, 99	0
All	All	961/979 (98%)	1.25	243 (25%)  	22, 45, 90, 146	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	THR	9.5
1	A	289	LEU	8.1
2	B	355	ALA	7.2
2	B	92	LEU	6.8
2	B	425	LEU	6.4
1	A	552	VAL	6.3
1	A	282	LEU	6.0
2	B	357	MET	5.9
1	A	225	PRO	5.9
1	A	292	VAL	5.9
1	A	285	GLY	5.7
1	A	542	ILE	5.7
1	A	543	GLY	5.5
1	A	546	GLU	5.5
2	B	360	ALA	5.4
2	B	212	TRP	5.2
1	A	280	SER	5.1
2	B	88	TRP	5.1
1	A	301	LEU	5.0
2	B	316	GLY	5.0
2	B	241	VAL	4.9
1	A	91	GLN	4.8
2	B	195	ILE	4.8
2	B	68	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	92	LEU	4.7
1	A	65	LYS	4.7
1	A	544	GLY	4.7
1	A	69	THR	4.7
1	A	288	ALA	4.6
1	A	3	SER	4.6
2	B	242	GLN	4.5
1	A	286	THR	4.5
1	A	90	VAL	4.5
2	B	210	LEU	4.5
2	B	361	HIS	4.4
1	A	226	PRO	4.3
2	B	213	GLY	4.3
2	B	226	PRO	4.3
1	A	217	PRO	4.2
1	A	253	THR	4.2
1	A	135	ILE	4.2
2	B	318	TYR	4.2
1	A	218	ASP	4.2
1	A	24	TRP	4.2
2	B	301	LEU	4.2
1	A	296	THR	4.1
2	B	7	THR	4.1
1	A	66	LYS	4.0
1	A	255	ASN	4.0
1	A	216	THR	4.0
1	A	541	GLY	4.0
2	B	67	ASP	4.0
1	A	134	SER	4.0
2	B	358	ARG	3.9
2	B	359	GLY	3.9
1	A	215	THR	3.9
1	A	548	VAL	3.9
1	A	449	GLU	3.9
2	B	356	ARG	3.9
1	A	283	LEU	3.9
2	B	196	GLY	3.9
1	A	279	LEU	3.8
1	A	554	ALA	3.8
2	B	69	THR	3.8
1	A	268	SER	3.8
2	B	85	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	179	VAL	3.7
2	B	428	GLN	3.7
1	A	114	ALA	3.7
1	A	102	LYS	3.7
2	B	354	TYR	3.6
2	B	232	TYR	3.6
2	B	236	PRO	3.6
1	A	553	SER	3.5
2	B	273	GLY	3.5
1	A	547	GLN	3.5
2	B	313	PRO	3.5
1	A	291	GLU	3.5
1	A	203	GLU	3.4
1	A	169	GLU	3.4
2	B	66	LYS	3.3
1	A	220	LYS	3.3
1	A	302	GLU	3.3
2	B	15	GLY	3.3
1	A	142	ILE	3.3
1	A	299	ALA	3.3
1	A	61	PHE	3.3
1	A	419	THR	3.3
2	B	86	ASP	3.2
2	B	227	PHE	3.2
1	A	194	GLU	3.2
2	B	285	GLY	3.2
1	A	31	ILE	3.2
1	A	167	ILE	3.2
2	B	8	VAL	3.2
1	A	276	VAL	3.2
2	B	426	TRP	3.1
2	B	200	THR	3.1
1	A	250	ASP	3.1
1	A	311	LYS	3.1
1	A	304	ALA	3.1
1	A	212	TRP	3.1
2	B	427	TYR	3.1
1	A	221	HIS	3.1
2	B	296	THR	3.1
2	B	95	PRO	3.1
1	A	222	GLN	3.0
2	B	64	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	227	PHE	3.0
2	B	312	GLU	3.0
2	B	140	PRO	3.0
2	B	240	THR	3.0
1	A	295	LEU	3.0
1	A	68	SER	3.0
2	B	321	PRO	3.0
1	A	33	ALA	3.0
2	B	202	ILE	3.0
2	B	139	THR	2.9
2	B	231	GLY	2.9
2	B	237	ASP	2.9
1	A	251	SER	2.9
1	A	140	PRO	2.9
2	B	176	PRO	2.9
1	A	67	ASP	2.8
1	A	237	ASP	2.8
1	A	88	TRP	2.8
2	B	89	GLU	2.8
1	A	32	LYS	2.8
1	A	200	THR	2.8
2	B	305	GLU	2.8
2	B	87	PHE	2.8
1	A	254	VAL	2.8
1	A	70	LYS	2.7
1	A	116	PHE	2.7
1	A	223	LYS	2.7
1	A	281	LYS	2.7
1	A	450	THR	2.7
1	A	246	LEU	2.7
1	A	224	GLU	2.7
1	A	177	ASP	2.7
1	A	277	ARG	2.7
1	A	35	VAL	2.7
2	B	315	HIS	2.7
2	B	193	LEU	2.7
1	A	75	VAL	2.7
1	A	359	GLY	2.6
1	A	110	ASP	2.6
2	B	177	ASP	2.6
1	A	174	GLN	2.6
2	B	272	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	15	GLY	2.6
1	A	357	MET	2.6
1	A	185	ASP	2.6
2	B	6	GLU	2.6
2	B	194	GLU	2.6
1	A	141	GLY	2.6
1	A	183	TYR	2.6
1	A	71	TRP	2.6
2	B	239	TRP	2.6
1	A	74	LEU	2.6
2	B	228	LEU	2.6
2	B	282	LEU	2.5
1	A	64	LYS	2.5
2	B	191	SER	2.5
1	A	214	LEU	2.5
1	A	228	LEU	2.5
1	A	257	ILE	2.5
2	B	229	TRP	2.5
1	A	447	ASN	2.5
2	B	314	VAL	2.5
2	B	422	LEU	2.5
1	A	63	ILE	2.5
1	A	89	GLU	2.4
1	A	284	ARG	2.4
1	A	334	GLN	2.4
1	A	184	MET	2.4
2	B	186	ASP	2.4
1	A	199	ARG	2.4
2	B	199	ARG	2.4
2	B	9	PRO	2.4
2	B	283	LEU	2.4
1	A	293	ILE	2.4
1	A	312	GLU	2.4
2	B	138	GLU	2.4
1	A	136	ASN	2.4
1	A	60	VAL	2.4
1	A	549	ASP	2.3
1	A	210	LEU	2.3
1	A	355	ALA	2.3
2	B	423	VAL	2.3
1	A	182	GLN	2.3
1	A	115	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	178	ILE	2.3
1	A	139	THR	2.3
2	B	175	ASN	2.3
2	B	230	MET	2.3
1	A	176	PRO	2.3
2	B	97	PRO	2.3
2	B	167	ILE	2.3
2	B	208	HIS	2.3
2	B	209	LEU	2.3
1	A	112	GLY	2.2
2	B	319	TYR	2.2
1	A	121	ASP	2.2
1	A	287	LYS	2.2
2	B	102	LYS	2.2
1	A	551	LEU	2.2
1	A	93	GLY	2.2
1	A	256	ASP	2.2
1	A	82	LYS	2.2
2	B	122	GLU	2.2
2	B	362	THR	2.2
1	A	44	GLU	2.1
2	B	207	GLN	2.1
1	A	358	ARG	2.1
1	A	529	GLU	2.1
1	A	137	ASN	2.1
1	A	519	ASN	2.1
1	A	17	ASP	2.1
1	A	131	THR	2.1
1	A	51	GLY	2.1
1	A	25	PRO	2.1
1	A	27	THR	2.1
2	B	238	LYS	2.1
1	A	262	GLY	2.1
2	B	106	VAL	2.1
1	A	260	LEU	2.1
2	B	320	ASP	2.1
1	A	300	GLU	2.0
1	A	207	GLN	2.0
1	A	193	LEU	2.0
1	A	192	ASP	2.0
2	B	110	ASP	2.0
2	B	204	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	22	LYS	2.0
1	A	30	LYS	2.0
2	B	11	LYS	2.0
2	B	172	LYS	2.0
2	B	173	LYS	2.0
1	A	195	ILE	2.0
1	A	213	GLY	2.0
1	A	420	PRO	2.0
1	A	72	ARG	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
3	SO4	A	556	5/5	0.78	0.14	65,65,66,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.