



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:27 PM UTC

PDB ID : 1QQC / pdb_00001qqc
Title : CRYSTAL STRUCTURE OF AN ARCHAEBACTERIAL DNA POLYMERASE D.TOK
Authors : Zhao, Y.; Jeruzalmi, D.; Leighton, L.; Lasken, R.; Kuriyan, J.
Deposited on : 1999-06-02
Resolution : 2.60 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

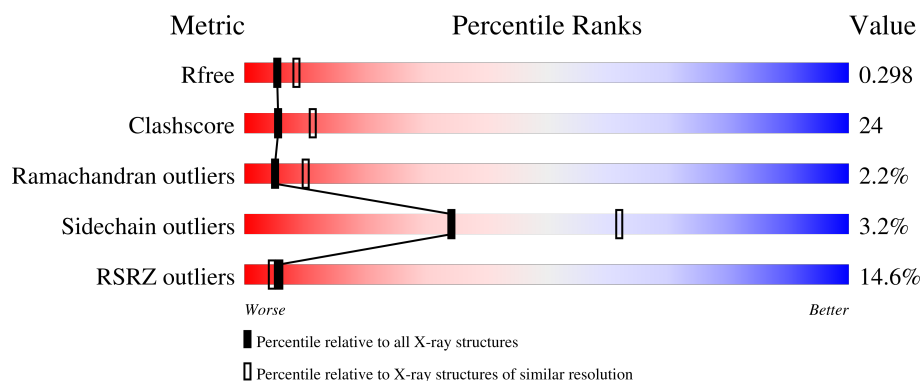
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	773	14% 57% 33% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6167 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 DNA POLYMERASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	0	0
			6029	3870	1032	1112	15			

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



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Mg 2	0	0

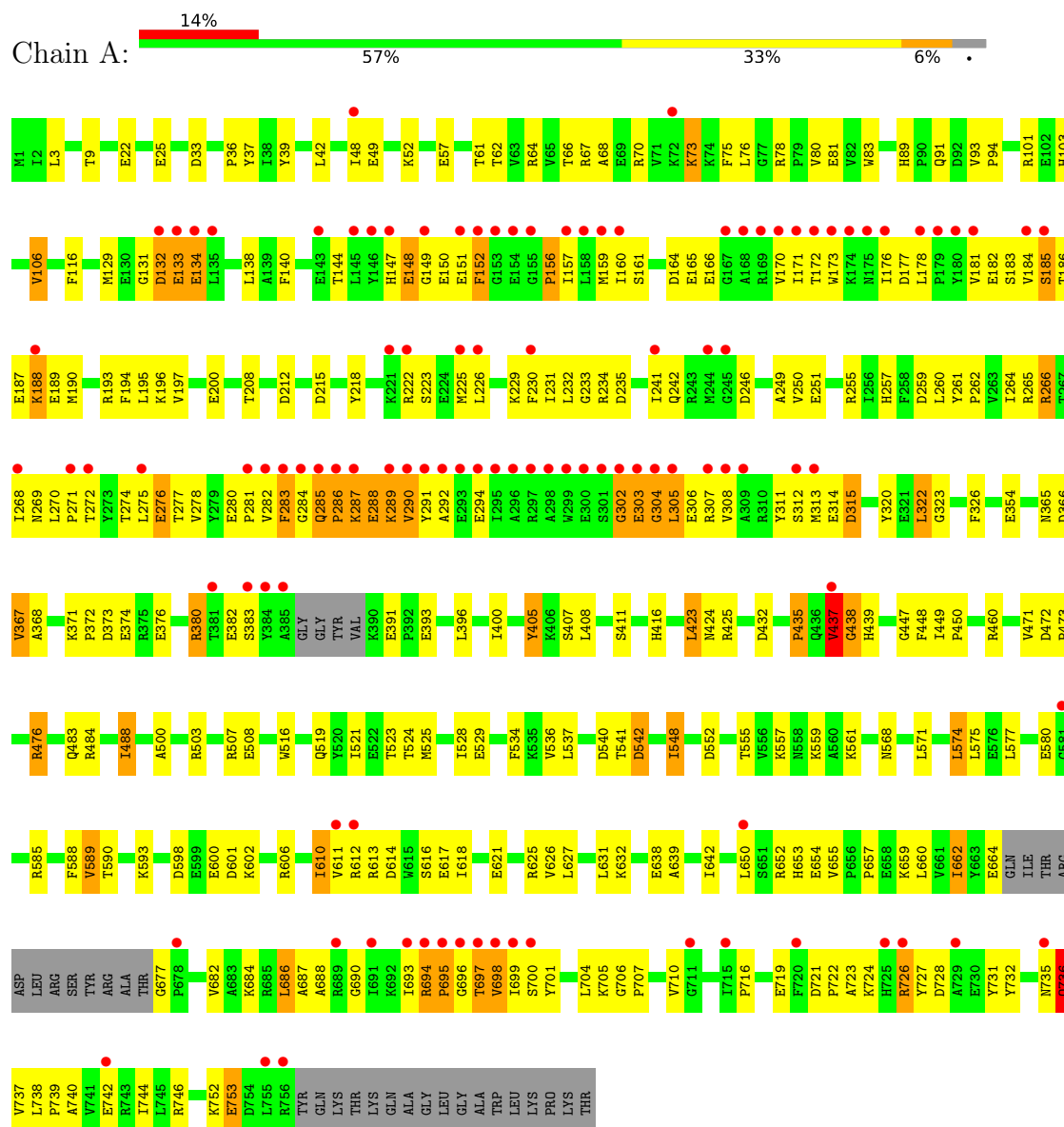
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total 116	O 116	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: DNA POLYMERASE II



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.10Å 107.60Å 155.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.3 (50.00-2.60) 92.1 (50.00-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.47 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.295 0.248 , 0.298	Depositor DCC
R_{free} test set	3212 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6167	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: MG, 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	0.51	0/6164	1.15	57/8324 (0.7%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	736	GLN	N-CA-C	11.03	127.51	111.96
1	A	289	LYS	N-CA-C	10.96	124.60	108.60
1	A	292	ALA	N-CA-C	-10.74	96.22	113.19
1	A	285	GLN	CA-C-N	9.40	129.24	120.21
1	A	285	GLN	C-N-CA	9.40	129.24	120.21
1	A	695	PRO	N-CA-C	8.56	124.56	113.86
1	A	304	GLY	N-CA-C	-8.51	92.28	115.86
1	A	697	THR	N-CA-C	8.26	122.44	109.81
1	A	133	GLU	N-CA-C	8.05	121.42	110.55
1	A	33	ASP	N-CA-C	7.42	122.06	112.26
1	A	383	SER	N-CA-C	7.33	119.79	110.33
1	A	287	LYS	N-CA-C	-7.08	98.96	108.74
1	A	589	VAL	N-CA-C	7.06	118.02	111.45
1	A	132	ASP	N-CA-C	-6.90	102.99	112.03
1	A	286	PRO	N-CA-C	6.78	120.72	111.22
1	A	706	GLY	CA-C-N	6.71	128.23	119.84
1	A	706	GLY	C-N-CA	6.71	128.23	119.84
1	A	284	GLY	N-CA-C	6.68	129.01	113.18
1	A	400	ILE	N-CA-C	6.65	117.48	108.17
1	A	677	GLY	CA-C-N	6.65	126.10	118.85
1	A	677	GLY	C-N-CA	6.65	126.10	118.85
1	A	613	ARG	N-CA-C	-6.60	104.82	114.39
1	A	437	VAL	N-CA-CB	-6.41	104.89	112.39
1	A	25	GLU	N-CA-C	6.15	119.56	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	737	VAL	N-CA-C	6.13	116.30	110.42
1	A	548	ILE	N-CA-C	-6.07	101.11	107.60
1	A	610	ILE	N-CA-C	6.02	116.19	108.12
1	A	103	HIS	N-CA-C	-5.99	101.50	110.24
1	A	698	VAL	CA-C-N	-5.91	115.60	123.17
1	A	698	VAL	C-N-CA	-5.91	115.60	123.17
1	A	368	ALA	N-CA-C	5.91	117.51	110.07
1	A	223	SER	N-CA-C	-5.78	107.47	114.75
1	A	322	LEU	N-CA-C	-5.75	104.62	111.69
1	A	283	PHE	N-CA-C	5.73	123.00	110.80
1	A	64	ARG	N-CA-C	5.71	117.29	109.18
1	A	57	GLU	N-CA-C	5.67	118.01	109.23
1	A	542	ASP	N-CA-C	5.66	119.63	111.02
1	A	391	GLU	CA-C-N	5.64	126.08	119.99
1	A	391	GLU	C-N-CA	5.64	126.08	119.99
1	A	687	ALA	N-CA-C	-5.64	106.48	113.19
1	A	315	ASP	N-CA-C	-5.62	105.06	111.07
1	A	374	GLU	N-CA-C	5.62	117.85	111.11
1	A	215	ASP	N-CA-C	5.60	118.11	111.33
1	A	631	LEU	N-CA-C	5.56	118.53	111.69
1	A	288	GLU	N-CA-C	5.52	118.39	109.40
1	A	686	LEU	N-CA-C	-5.46	106.66	113.55
1	A	246	ASP	N-CA-C	-5.33	106.45	113.17
1	A	438	GLY	N-CA-C	5.32	125.78	113.18
1	A	437	VAL	N-CA-C	5.24	116.58	111.91
1	A	753	GLU	N-CA-C	5.20	117.69	111.71
1	A	726	ARG	N-CA-C	-5.20	102.50	110.14
1	A	73	LYS	N-CA-C	5.19	116.17	108.86
1	A	294	GLU	N-CA-C	-5.17	105.76	111.71
1	A	150	GLU	N-CA-C	5.14	117.31	110.53
1	A	106	VAL	N-CA-C	5.07	114.88	107.37
1	A	265	ARG	N-CA-C	-5.06	107.39	113.21
1	A	303	GLU	N-CA-C	5.03	121.51	110.80

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	6029	0	5991	284	0
2	A	20	0	0	0	0
3	A	2	0	0	0	0
4	A	116	0	0	5	0
All	All	6167	0	5991	284	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 24.

All (284) 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:176:ILE:HG12	1:A:305:LEU:HD21	1.42	1.00
1:A:290:VAL:HG11	1:A:697:THR:HA	1.48	0.94
1:A:694:ARG:HB3	1:A:695:PRO:HD2	1.48	0.92
1:A:159:MET:HG2	1:A:172:THR:CG2	2.01	0.91
1:A:437:VAL:HG13	1:A:439:HIS:CD2	2.05	0.91
1:A:460:ARG:HH21	1:A:483:GLN:NE2	1.69	0.90
1:A:460:ARG:HE	1:A:483:GLN:HE21	1.23	0.87
1:A:75:PHE:HD1	1:A:367:VAL:HG12	1.39	0.85
1:A:476:ARG:HB2	1:A:476:ARG:HH11	1.42	0.84
1:A:303:GLU:C	1:A:305:LEU:H	1.84	0.84
1:A:697:THR:HG22	1:A:698:VAL:H	1.40	0.84
1:A:159:MET:HG2	1:A:172:THR:HG22	1.59	0.83
1:A:161:SER:HB3	1:A:170:VAL:HG22	1.59	0.83
1:A:196:LYS:O	1:A:200:GLU:HG3	1.80	0.81
1:A:460:ARG:HH21	1:A:483:GLN:HE22	1.26	0.81
1:A:188:LYS:HE2	1:A:226:LEU:HG	1.62	0.80
1:A:75:PHE:CD1	1:A:367:VAL:HG12	2.17	0.79
1:A:521:ILE:HD11	1:A:541:THR:O	1.83	0.79
1:A:697:THR:HG22	1:A:698:VAL:N	1.98	0.78
1:A:264:ILE:HD13	1:A:278:VAL:HG11	1.65	0.78
1:A:285:GLN:HB2	1:A:286:PRO:HD2	1.65	0.77
1:A:571:LEU:HD22	1:A:575:LEU:HD11	1.68	0.76
1:A:627:LEU:HD21	1:A:744:ILE:HD13	1.66	0.75
1:A:148:GLU:CB	1:A:694:ARG:HH12	2.00	0.75
1:A:612:ARG:NH2	1:A:735:ASN:OD1	2.20	0.74
1:A:305:LEU:HD23	1:A:306:GLU:N	2.03	0.74
1:A:303:GLU:C	1:A:305:LEU:N	2.44	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:VAL:CG1	1:A:697:THR:HA	2.18	0.73
1:A:78:ARG:HG2	1:A:425:ARG:HH22	1.54	0.72
1:A:22:GLU:HA	1:A:133:GLU:OE2	1.90	0.71
1:A:694:ARG:HB3	1:A:695:PRO:CD	2.20	0.71
1:A:186:THR:HG22	1:A:189:GLU:HG2	1.73	0.70
1:A:303:GLU:HG2	1:A:306:GLU:HB2	1.74	0.70
1:A:73:LYS:HD3	1:A:367:VAL:HG23	1.73	0.70
1:A:697:THR:CG2	1:A:698:VAL:H	2.05	0.69
1:A:574:LEU:HD12	1:A:574:LEU:H	1.57	0.69
1:A:291:TYR:HE1	1:A:311:TYR:CG	2.09	0.69
1:A:460:ARG:NE	1:A:483:GLN:HE21	1.90	0.69
1:A:187:GLU:HG3	1:A:226:LEU:HD21	1.73	0.68
1:A:476:ARG:HB2	1:A:476:ARG:NH1	2.07	0.68
1:A:36:PRO:HG3	1:A:116:PHE:CE1	2.28	0.68
1:A:159:MET:HG2	1:A:172:THR:HG21	1.75	0.68
1:A:260:LEU:HD21	1:A:323:GLY:HA2	1.76	0.68
1:A:291:TYR:HE1	1:A:311:TYR:CD1	2.11	0.67
1:A:290:VAL:HB	1:A:698:VAL:HG23	1.77	0.67
1:A:437:VAL:CG1	1:A:439:HIS:CD2	2.77	0.67
1:A:78:ARG:NE	1:A:425:ARG:NH2	2.43	0.67
1:A:271:PRO:HG2	1:A:272:THR:H	1.59	0.67
1:A:274:THR:HG22	1:A:276:GLU:OE2	1.94	0.67
1:A:705:LYS:N	4:A:2084:HOH:O	2.27	0.66
1:A:289:LYS:CG	1:A:290:VAL:H	2.08	0.66
1:A:181:VAL:HG12	1:A:182:GLU:N	2.11	0.66
1:A:277:THR:O	1:A:281:PRO:HD2	1.94	0.66
1:A:184:VAL:HG12	1:A:185:SER:N	2.11	0.65
1:A:372:PRO:HG3	1:A:380:ARG:NH1	2.11	0.65
1:A:261:TYR:HB3	1:A:262:PRO:HD3	1.78	0.65
1:A:93:VAL:HB	1:A:94:PRO:HD3	1.79	0.64
1:A:652:ARG:O	1:A:654:GLU:HG3	1.98	0.64
1:A:664:GLU:HG2	1:A:699:ILE:HG22	1.79	0.64
1:A:188:LYS:H	1:A:188:LYS:HD2	1.63	0.64
1:A:39:TYR:CE2	1:A:73:LYS:HE3	2.33	0.63
1:A:160:ILE:HG23	1:A:171:ILE:CG2	2.29	0.63
1:A:160:ILE:HG23	1:A:171:ILE:HG23	1.80	0.63
1:A:460:ARG:NH2	1:A:483:GLN:NE2	2.45	0.63
1:A:39:TYR:CZ	1:A:73:LYS:HE3	2.33	0.63
1:A:195:LEU:HD21	1:A:230:PHE:CD1	2.34	0.63
1:A:91:GLN:O	1:A:94:PRO:HD2	1.98	0.62
1:A:280:GLU:N	1:A:281:PRO:HD2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:VAL:CG1	1:A:439:HIS:HD2	2.12	0.62
1:A:571:LEU:HD13	1:A:575:LEU:CD1	2.29	0.62
1:A:552:ASP:HB3	1:A:555:THR:OG1	1.99	0.62
1:A:416:HIS:HD2	1:A:432:ASP:OD1	1.83	0.62
1:A:574:LEU:HD12	1:A:574:LEU:N	2.15	0.61
1:A:618:ILE:HD12	1:A:655:VAL:HG11	1.82	0.61
1:A:176:ILE:CG1	1:A:305:LEU:HD21	2.26	0.61
1:A:616:SER:CB	1:A:736:GLN:NE2	2.64	0.61
1:A:688:ALA:C	1:A:690:GLY:H	2.08	0.61
1:A:638:GLU:O	1:A:642:ILE:HG13	2.00	0.61
1:A:437:VAL:O	1:A:439:HIS:N	2.32	0.61
1:A:285:GLN:CB	1:A:286:PRO:HD2	2.28	0.60
1:A:101:ARG:NH1	4:A:2009:HOH:O	2.33	0.60
1:A:259:ASP:O	1:A:262:PRO:HD2	2.00	0.60
1:A:752:LYS:HG3	1:A:753:GLU:HG3	1.84	0.60
1:A:287:LYS:HG2	1:A:288:GLU:H	1.66	0.60
1:A:287:LYS:HG2	1:A:288:GLU:N	2.15	0.60
1:A:302:GLY:O	1:A:303:GLU:HG3	2.02	0.59
1:A:616:SER:HB3	1:A:736:GLN:NE2	2.18	0.59
1:A:234:ARG:HG3	1:A:255:ARG:NH1	2.17	0.59
1:A:598:ASP:OD1	1:A:602:LYS:HB3	2.03	0.59
1:A:738:LEU:O	1:A:742:GLU:HG3	2.03	0.59
1:A:188:LYS:HG3	1:A:226:LEU:HB3	1.83	0.58
1:A:519:GLN:O	1:A:523:THR:HG23	2.03	0.58
1:A:78:ARG:NH2	4:A:2054:HOH:O	2.35	0.58
1:A:664:GLU:HA	1:A:699:ILE:CG2	2.33	0.58
1:A:78:ARG:NE	1:A:425:ARG:HH21	2.01	0.58
1:A:186:THR:CG2	1:A:189:GLU:HG2	2.33	0.58
1:A:76:LEU:O	1:A:78:ARG:HG3	2.04	0.58
1:A:144:THR:HG23	1:A:156:PRO:O	2.04	0.57
1:A:305:LEU:HD23	1:A:305:LEU:C	2.30	0.57
1:A:704:LEU:HD22	1:A:726:ARG:O	2.04	0.57
1:A:731:TYR:CZ	1:A:735:ASN:ND2	2.67	0.57
1:A:282:VAL:HG21	1:A:322:LEU:HD22	1.86	0.56
1:A:132:ASP:OD1	1:A:132:ASP:O	2.23	0.56
1:A:172:THR:O	1:A:183:SER:HA	2.06	0.56
1:A:78:ARG:HE	1:A:425:ARG:NH2	2.04	0.56
1:A:289:LYS:HD3	1:A:290:VAL:N	2.21	0.56
1:A:290:VAL:HG11	1:A:697:THR:CA	2.29	0.55
1:A:157:ILE:O	1:A:190:MET:HE1	2.06	0.55
1:A:752:LYS:HG3	1:A:753:GLU:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:ARG:HD3	1:A:746:ARG:O	2.07	0.55
1:A:148:GLU:CB	1:A:694:ARG:NH1	2.70	0.55
1:A:188:LYS:H	1:A:188:LYS:CD	2.20	0.55
1:A:448:PHE:CD2	1:A:449:ILE:HD12	2.42	0.54
1:A:724:LYS:HE2	4:A:2083:HOH:O	2.06	0.54
1:A:593:LYS:HA	1:A:606:ARG:O	2.06	0.54
1:A:241:ILE:HG12	1:A:250:VAL:HG22	1.90	0.54
1:A:508:GLU:OE2	1:A:508:GLU:N	2.39	0.54
1:A:589:VAL:HG12	1:A:590:THR:HG23	1.89	0.54
1:A:188:LYS:HD2	1:A:188:LYS:N	2.22	0.54
1:A:650:LEU:HD21	1:A:732:TYR:HB3	1.90	0.54
1:A:188:LYS:HG3	1:A:226:LEU:CG	2.38	0.54
1:A:437:VAL:HG13	1:A:437:VAL:O	2.08	0.54
1:A:181:VAL:CG1	1:A:182:GLU:N	2.70	0.54
1:A:289:LYS:CD	1:A:290:VAL:H	2.21	0.54
1:A:396:LEU:HD11	1:A:585:ARG:HD3	1.89	0.53
1:A:287:LYS:NZ	1:A:315:ASP:OD2	2.42	0.53
1:A:571:LEU:HB3	1:A:575:LEU:HD11	1.89	0.53
1:A:282:VAL:HG12	1:A:283:PHE:CD2	2.43	0.53
1:A:612:ARG:HH22	1:A:735:ASN:CG	2.15	0.53
1:A:138:LEU:C	1:A:138:LEU:HD23	2.34	0.53
1:A:524:THR:HG21	1:A:577:LEU:HD11	1.89	0.53
1:A:627:LEU:HD21	1:A:744:ILE:CD1	2.37	0.53
1:A:222:ARG:O	1:A:226:LEU:HD13	2.09	0.53
1:A:484:ARG:HG2	1:A:484:ARG:HH11	1.74	0.53
1:A:752:LYS:HG3	1:A:753:GLU:N	2.24	0.52
1:A:699:ILE:HG23	1:A:699:ILE:O	2.09	0.52
1:A:528:ILE:HG12	1:A:534:PHE:HB2	1.91	0.52
1:A:611:VAL:HG12	1:A:611:VAL:O	2.10	0.52
1:A:165:GLU:HG2	1:A:320:TYR:OH	2.09	0.52
1:A:187:GLU:O	1:A:190:MET:HB3	2.09	0.52
1:A:614:ASP:HB3	1:A:662:ILE:HD11	1.90	0.52
1:A:148:GLU:CA	1:A:694:ARG:HH12	2.22	0.52
1:A:147:HIS:O	1:A:148:GLU:C	2.52	0.52
1:A:80:VAL:HG22	1:A:81:GLU:N	2.25	0.51
1:A:571:LEU:HD13	1:A:575:LEU:HD12	1.92	0.51
1:A:660:LEU:HD22	1:A:732:TYR:CD2	2.45	0.51
1:A:289:LYS:HG2	1:A:290:VAL:H	1.73	0.51
1:A:521:ILE:CD1	1:A:541:THR:O	2.56	0.51
1:A:70:ARG:HE	1:A:81:GLU:CD	2.19	0.51
1:A:686:LEU:C	1:A:688:ALA:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ILE:HD11	1:A:559:LYS:HG2	1.93	0.51
1:A:140:PHE:HA	1:A:161:SER:O	2.11	0.50
1:A:278:VAL:O	1:A:282:VAL:HG23	2.11	0.50
1:A:291:TYR:CE1	1:A:311:TYR:CD1	2.96	0.50
1:A:382:GLU:O	1:A:507:ARG:NH2	2.43	0.50
1:A:275:LEU:HD13	1:A:275:LEU:O	2.11	0.50
1:A:525:MET:HE3	1:A:536:VAL:HG11	1.93	0.50
1:A:48:ILE:HG13	1:A:49:GLU:N	2.26	0.50
1:A:48:ILE:HD13	1:A:83:TRP:CH2	2.47	0.50
1:A:627:LEU:CD2	1:A:744:ILE:HD13	2.37	0.50
1:A:9:THR:OG1	1:A:89:HIS:HE1	1.94	0.50
1:A:721:ASP:C	1:A:723:ALA:H	2.19	0.50
1:A:290:VAL:HG13	1:A:696:GLY:O	2.11	0.50
1:A:524:THR:CG2	1:A:577:LEU:HD11	2.42	0.50
1:A:277:THR:O	1:A:281:PRO:CD	2.59	0.49
1:A:285:GLN:HB2	1:A:286:PRO:CD	2.39	0.49
1:A:698:VAL:HG12	1:A:698:VAL:O	2.11	0.49
1:A:91:GLN:C	1:A:94:PRO:HD2	2.37	0.49
1:A:289:LYS:CG	1:A:290:VAL:N	2.75	0.49
1:A:484:ARG:O	1:A:488:ILE:HD12	2.12	0.49
1:A:177:ASP:O	1:A:306:GLU:OE2	2.30	0.49
1:A:393:GLU:HG3	1:A:537:LEU:HD23	1.94	0.49
1:A:89:HIS:CD2	1:A:91:GLN:H	2.31	0.48
1:A:144:THR:HG21	1:A:218:TYR:OH	2.13	0.48
1:A:571:LEU:HB3	1:A:575:LEU:CD1	2.42	0.48
1:A:716:PRO:HD2	1:A:719:GLU:OE1	2.12	0.48
1:A:731:TYR:OH	1:A:735:ASN:ND2	2.46	0.48
1:A:423:LEU:CD2	1:A:424:ASN:ND2	2.76	0.48
1:A:662:ILE:O	1:A:700:SER:HA	2.14	0.48
1:A:557:LYS:O	1:A:561:LYS:HG2	2.14	0.48
1:A:193:ARG:O	1:A:197:VAL:HG23	2.13	0.48
1:A:164:ASP:OD1	1:A:165:GLU:N	2.47	0.48
1:A:184:VAL:CG1	1:A:185:SER:N	2.75	0.48
1:A:197:VAL:HA	1:A:200:GLU:OE1	2.14	0.48
1:A:616:SER:CB	1:A:736:GLN:HE21	2.26	0.47
1:A:735:ASN:O	1:A:739:PRO:HG3	2.13	0.47
1:A:148:GLU:HA	1:A:694:ARG:NH1	2.29	0.47
1:A:372:PRO:HG2	1:A:500:ALA:O	2.14	0.47
1:A:610:ILE:CG2	1:A:612:ARG:HB2	2.44	0.47
1:A:184:VAL:HG12	1:A:185:SER:H	1.77	0.47
1:A:188:LYS:HG3	1:A:226:LEU:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:VAL:HG12	1:A:710:VAL:O	2.14	0.47
1:A:371:LYS:HG3	1:A:503:ARG:NH1	2.30	0.47
1:A:275:LEU:HD13	1:A:275:LEU:C	2.39	0.47
1:A:616:SER:OG	1:A:736:GLN:NE2	2.47	0.47
1:A:660:LEU:HB3	1:A:732:TYR:CE2	2.50	0.46
1:A:601:ASP:OD2	1:A:632:LYS:HE3	2.15	0.46
1:A:408:LEU:O	1:A:411:SER:HB3	2.15	0.46
1:A:448:PHE:HD2	1:A:449:ILE:HD12	1.80	0.46
1:A:160:ILE:CG2	1:A:171:ILE:HG23	2.44	0.46
1:A:232:LEU:O	1:A:255:ARG:NH1	2.49	0.46
1:A:264:ILE:C	1:A:266:ARG:H	2.23	0.46
1:A:484:ARG:HG2	1:A:484:ARG:NH1	2.31	0.46
1:A:568:ASN:HD22	1:A:571:LEU:HD12	1.80	0.46
1:A:437:VAL:CG1	1:A:437:VAL:O	2.63	0.46
1:A:617:GLU:HB3	1:A:659:LYS:O	2.16	0.46
1:A:66:THR:HG22	1:A:67:ARG:HG3	1.96	0.45
1:A:160:ILE:HD11	1:A:194:PHE:CE1	2.52	0.45
1:A:3:LEU:HD23	1:A:129:MET:HE1	1.98	0.45
1:A:305:LEU:CD2	1:A:306:GLU:N	2.78	0.45
1:A:173:TRP:HA	1:A:184:VAL:O	2.17	0.45
1:A:405:TYR:HD1	1:A:542:ASP:O	2.00	0.45
1:A:148:GLU:CA	1:A:694:ARG:NH1	2.79	0.45
1:A:37:TYR:CD1	1:A:37:TYR:C	2.95	0.45
1:A:638:GLU:OE2	1:A:638:GLU:HA	2.16	0.45
1:A:694:ARG:CB	1:A:695:PRO:HD2	2.33	0.45
1:A:626:VAL:HG13	1:A:639:ALA:HB1	1.99	0.44
1:A:447:GLY:C	1:A:450:PRO:HD2	2.42	0.44
1:A:42:LEU:N	1:A:42:LEU:HD12	2.32	0.44
1:A:472:ASP:HA	1:A:473:PRO:HD2	1.82	0.44
1:A:164:ASP:C	1:A:166:GLU:N	2.74	0.44
1:A:304:GLY:O	1:A:307:ARG:HB3	2.17	0.44
1:A:529:GLU:HG2	1:A:534:PHE:O	2.18	0.44
1:A:151:GLU:O	1:A:152:PHE:C	2.61	0.44
1:A:588:PHE:CD1	1:A:588:PHE:N	2.85	0.44
1:A:682:VAL:O	1:A:686:LEU:HB2	2.18	0.44
1:A:187:GLU:HG3	1:A:226:LEU:CD2	2.44	0.44
1:A:580:GLU:C	1:A:580:GLU:CD	2.86	0.43
1:A:188:LYS:HA	1:A:226:LEU:HD23	2.00	0.43
1:A:303:GLU:HB3	1:A:304:GLY:H	1.68	0.43
1:A:621:GLU:O	1:A:625:ARG:HG3	2.18	0.43
1:A:52:LYS:HE2	1:A:68:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:THR:CG2	1:A:276:GLU:OE2	2.65	0.43
1:A:686:LEU:C	1:A:688:ALA:N	2.76	0.43
1:A:289:LYS:CD	1:A:290:VAL:N	2.81	0.43
1:A:312:SER:C	1:A:314:GLU:N	2.75	0.43
1:A:688:ALA:C	1:A:690:GLY:N	2.70	0.43
1:A:178:LEU:HD12	1:A:181:VAL:HG21	2.00	0.43
1:A:208:THR:OG1	1:A:257:HIS:HE1	2.02	0.43
1:A:268:ILE:HG22	1:A:270:LEU:HG	2.00	0.43
1:A:699:ILE:HG12	1:A:701:TYR:HD2	1.83	0.43
1:A:233:GLY:C	1:A:235:ASP:H	2.28	0.42
1:A:373:ASP:OD2	1:A:376:GLU:HG3	2.19	0.42
1:A:449:ILE:HB	1:A:450:PRO:HD3	2.01	0.42
1:A:187:GLU:CG	1:A:226:LEU:HD21	2.45	0.42
1:A:738:LEU:C	1:A:740:ALA:H	2.27	0.42
1:A:159:MET:HE1	1:A:308:VAL:HG12	2.02	0.42
1:A:276:GLU:CD	1:A:276:GLU:H	2.25	0.42
1:A:229:LYS:O	1:A:231:ILE:HG12	2.19	0.42
1:A:600:GLU:O	1:A:601:ASP:HB2	2.19	0.42
1:A:134:GLU:H	1:A:134:GLU:HG3	1.50	0.42
1:A:184:VAL:CG1	1:A:185:SER:H	2.31	0.42
1:A:313:MET:HE3	1:A:313:MET:HB2	1.86	0.42
1:A:269:ASN:O	1:A:270:LEU:HD23	2.20	0.42
1:A:280:GLU:N	1:A:281:PRO:CD	2.83	0.42
1:A:80:VAL:CG2	1:A:81:GLU:N	2.83	0.42
1:A:181:VAL:CG1	1:A:182:GLU:H	2.33	0.42
1:A:195:LEU:HD21	1:A:230:PHE:HD1	1.80	0.42
1:A:612:ARG:HH22	1:A:735:ASN:ND2	2.17	0.42
1:A:693:ILE:HG23	1:A:693:ILE:O	2.20	0.41
1:A:101:ARG:HA	1:A:106:VAL:HG11	2.02	0.41
1:A:614:ASP:HB3	1:A:662:ILE:CD1	2.51	0.41
1:A:312:SER:O	1:A:313:MET:C	2.64	0.41
1:A:73:LYS:HG2	1:A:365:ASN:OD1	2.21	0.41
1:A:161:SER:CB	1:A:170:VAL:HG22	2.42	0.41
1:A:322:LEU:O	1:A:326:PHE:HD1	2.03	0.41
1:A:735:ASN:OD1	1:A:735:ASN:O	2.39	0.41
1:A:686:LEU:HD12	1:A:686:LEU:HA	1.94	0.41
1:A:61:THR:HG22	1:A:62:THR:N	2.35	0.41
1:A:407:SER:O	1:A:411:SER:CB	2.69	0.41
1:A:460:ARG:CZ	1:A:483:GLN:HE21	2.34	0.41
1:A:650:LEU:HD21	1:A:732:TYR:CB	2.51	0.41
1:A:684:LYS:C	1:A:686:LEU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:HIS:HD2	1:A:91:GLN:H	1.69	0.41
1:A:276:GLU:OE1	1:A:289:LYS:HB2	2.21	0.41
1:A:212:ASP:HB3	1:A:249:ALA:HA	2.02	0.40
1:A:242:GLN:NE2	1:A:251:GLU:OE1	2.54	0.40
1:A:652:ARG:O	1:A:653:HIS:C	2.64	0.40
1:A:704:LEU:HA	4:A:2084:HOH:O	2.20	0.40
1:A:373:ASP:OD2	1:A:373:ASP:C	2.64	0.40
1:A:225:MET:H	1:A:225:MET:HG2	1.75	0.40
1:A:616:SER:HB3	1:A:736:GLN:HE22	1.85	0.40
1:A:460:ARG:HE	1:A:483:GLN:NE2	2.04	0.40
1:A:653:HIS:HA	1:A:727:TYR:CZ	2.57	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	734/773 (95%)	652 (89%)	66 (9%)	16 (2%)	5 10

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	GLU
1	A	152	PHE
1	A	185	SER
1	A	435	PRO
1	A	438	GLY
1	A	131	GLY
1	A	290	VAL
1	A	380	ARG
1	A	728	ASP
1	A	156	PRO

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Mol	Chain	Res	Type
1	A	694	ARG
1	A	707	PRO
1	A	722	PRO
1	A	657	PRO
1	A	302	GLY
1	A	149	GLY

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	630/670 (94%)	610 (97%)	20 (3%)	34 62

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	GLU
1	A	188	LYS
1	A	266	ARG
1	A	276	GLU
1	A	305	LEU
1	A	354	GLU
1	A	366	ASP
1	A	367	VAL
1	A	405	TYR
1	A	423	LEU
1	A	435	PRO
1	A	437	VAL
1	A	471	VAL
1	A	476	ARG
1	A	488	ILE
1	A	516	TRP
1	A	540	ASP
1	A	574	LEU
1	A	662	ILE
1	A	736	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	175	ASN
1	A	242	GLN
1	A	257	HIS
1	A	416	HIS
1	A	424	ASN
1	A	439	HIS
1	A	483	GLN
1	A	501	ASN
1	A	558	ASN
1	A	568	ASN
1	A	623	GLN
1	A	653	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1606	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	A	1130	-	4,4,4	0.19	0	6,6,6	0.11	0
2	SO4	A	1091	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	A	1487	-	4,4,4	0.21	0	6,6,6	0.10	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	740/773 (95%)	0.77	108 (14%) 6 4	22, 54, 111, 137	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	GLU	6.2
1	A	292	ALA	5.9
1	A	699	ILE	5.6
1	A	698	VAL	5.1
1	A	385	ALA	4.9
1	A	282	VAL	4.9
1	A	159	MET	4.7
1	A	384	TYR	4.6
1	A	132	ASP	4.6
1	A	696	GLY	4.5
1	A	697	THR	4.5
1	A	290	VAL	4.5
1	A	291	TYR	4.4
1	A	293	GLU	4.4
1	A	174	LYS	4.3
1	A	304	GLY	4.1
1	A	700	SER	3.9
1	A	151	GLU	3.9
1	A	299	TRP	3.9
1	A	155	GLY	3.8
1	A	296	ALA	3.8
1	A	153	GLY	3.7
1	A	295	ILE	3.6
1	A	383	SER	3.6
1	A	735	ASN	3.5
1	A	134	GLU	3.5
1	A	173	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	171	ILE	3.4
1	A	281	PRO	3.3
1	A	695	PRO	3.3
1	A	146	TYR	3.3
1	A	179	PRO	3.2
1	A	298	ALA	3.2
1	A	184	VAL	3.2
1	A	283	PHE	3.2
1	A	160	ILE	3.2
1	A	711	GLY	3.2
1	A	755	LEU	3.1
1	A	168	ALA	3.1
1	A	611	VAL	3.1
1	A	691	ILE	3.0
1	A	286	PRO	3.0
1	A	181	VAL	3.0
1	A	154	GLU	2.9
1	A	300	GLU	2.9
1	A	289	LYS	2.9
1	A	720	PHE	2.9
1	A	158	LEU	2.9
1	A	244	MET	2.9
1	A	693	ILE	2.9
1	A	284	GLY	2.9
1	A	178	LEU	2.9
1	A	152	PHE	2.9
1	A	308	VAL	2.9
1	A	180	TYR	2.8
1	A	650	LEU	2.8
1	A	176	ILE	2.8
1	A	275	LEU	2.8
1	A	305	LEU	2.8
1	A	287	LYS	2.7
1	A	694	ARG	2.7
1	A	285	GLN	2.7
1	A	48	ILE	2.7
1	A	301	SER	2.7
1	A	226	LEU	2.7
1	A	742	GLU	2.7
1	A	268	ILE	2.6
1	A	726	ARG	2.6
1	A	302	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	271	PRO	2.6
1	A	297	ARG	2.5
1	A	157	ILE	2.5
1	A	313	MET	2.5
1	A	241	ILE	2.5
1	A	170	VAL	2.4
1	A	185	SER	2.4
1	A	581	GLY	2.4
1	A	272	THR	2.3
1	A	303	GLU	2.3
1	A	312	SER	2.3
1	A	437	VAL	2.3
1	A	725	HIS	2.3
1	A	133	GLU	2.3
1	A	147	HIS	2.3
1	A	172	THR	2.3
1	A	145	LEU	2.3
1	A	222	ARG	2.3
1	A	678	PRO	2.2
1	A	72	LYS	2.2
1	A	612	ARG	2.2
1	A	729	ALA	2.2
1	A	175	ASN	2.2
1	A	135	LEU	2.2
1	A	245	GLY	2.2
1	A	309	ALA	2.1
1	A	169	ARG	2.1
1	A	188	LYS	2.1
1	A	149	GLY	2.1
1	A	167	GLY	2.1
1	A	230	PHE	2.1
1	A	143	GLU	2.1
1	A	689	ARG	2.1
1	A	221	LYS	2.0
1	A	381	THR	2.0
1	A	225	MET	2.0
1	A	307	ARG	2.0
1	A	715	ILE	2.0
1	A	756	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	MG	A	3031	1/1	0.59	0.35	111,111,111,111	0
3	MG	A	3030	1/1	0.70	0.24	100,100,100,100	0
2	SO4	A	1487	5/5	0.70	0.15	115,116,116,116	0
2	SO4	A	1606	5/5	0.78	0.18	118,119,119,120	0
2	SO4	A	1130	5/5	0.91	0.10	60,61,62,62	0
2	SO4	A	1091	5/5	0.96	0.07	45,46,49,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.