



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:10 PM UTC

PDB ID : 1R0K / pdb_00001r0k
Title : Crystal structure of 1-deoxy-D-xylulose 5-phosphate reductoisomerase from *Zymomonas mobilis*
Authors : Ricagno, S.; Grolle, S.; Bringer-Meyer, S.; Sahm, H.; Lindqvist, Y.; Schneider, G.
Deposited on : 2003-09-22
Resolution : 1.91 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

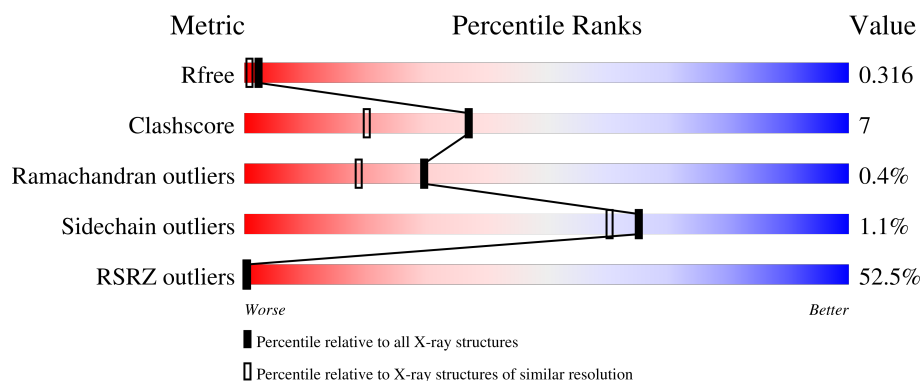
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	388	76% 84% 14% ..
1	B	388	43% 84% 14% ..
1	C	388	46% 81% 15% ..
1	D	388	41% 80% 17% ..

2 Entry composition [i](#)

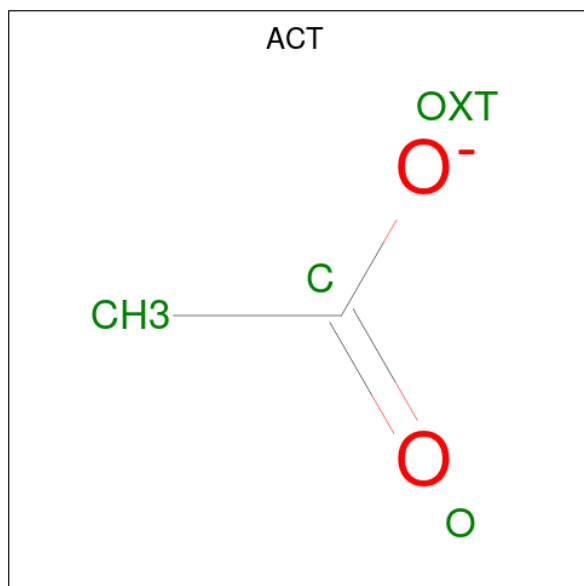
There are 3 unique types of molecules in this entry. The entry contains 12721 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2867	1806	498	547	16			
1	B	382	Total	C	N	O	S	0	0	0
			2885	1817	502	549	17			
1	C	379	Total	C	N	O	S	0	0	0
			2858	1801	496	545	16			
1	D	380	Total	C	N	O	S	0	0	0
			2871	1808	500	546	17			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	297	Total	O	0	0
			297	297		
3	B	349	Total	O	0	0
			349	349		
3	C	291	Total	O	0	0
			291	291		
3	D	287	Total	O	0	0
			287	287		

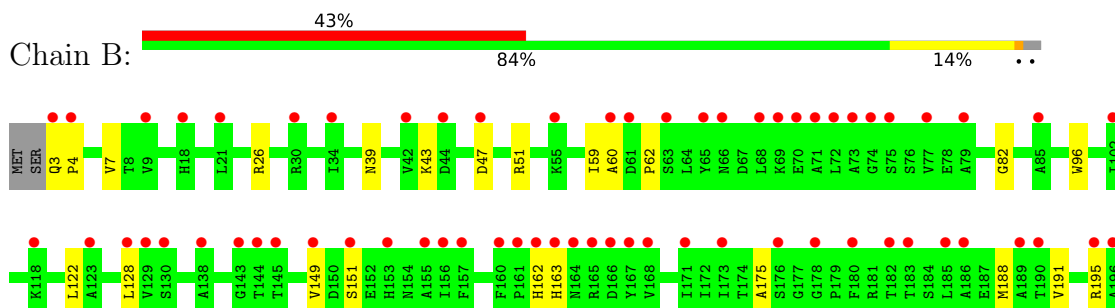
3 Residue-property plots

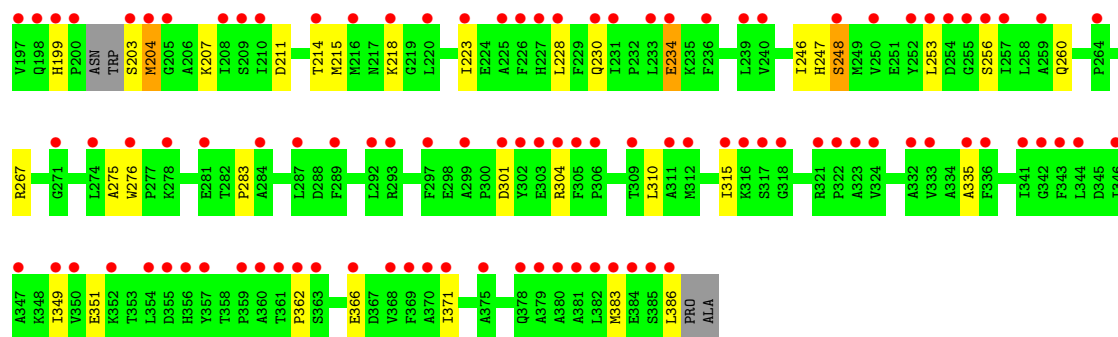
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

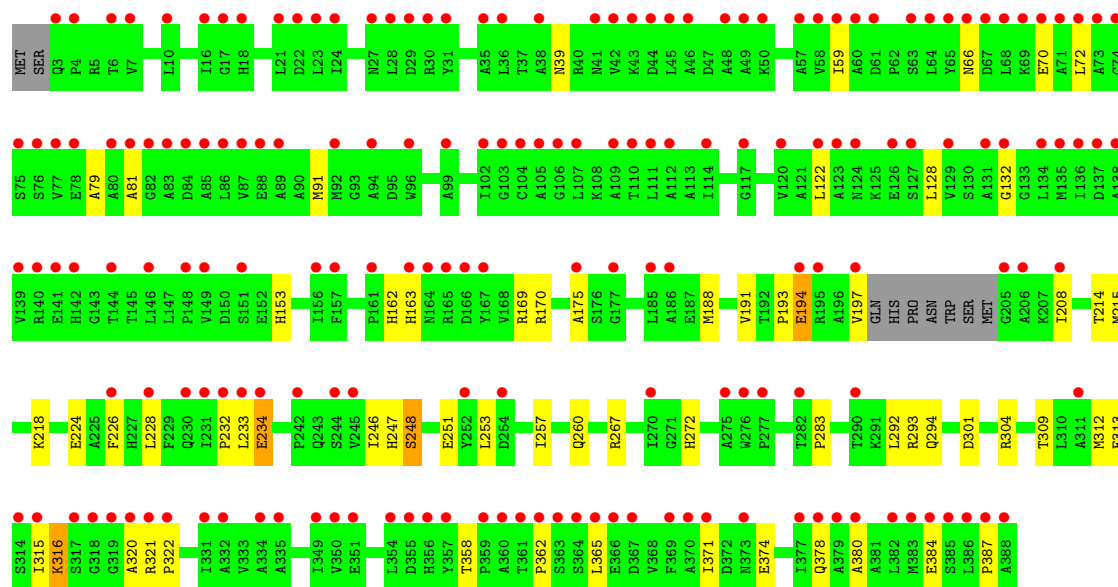
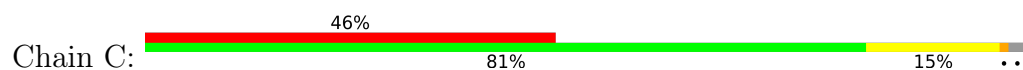


- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

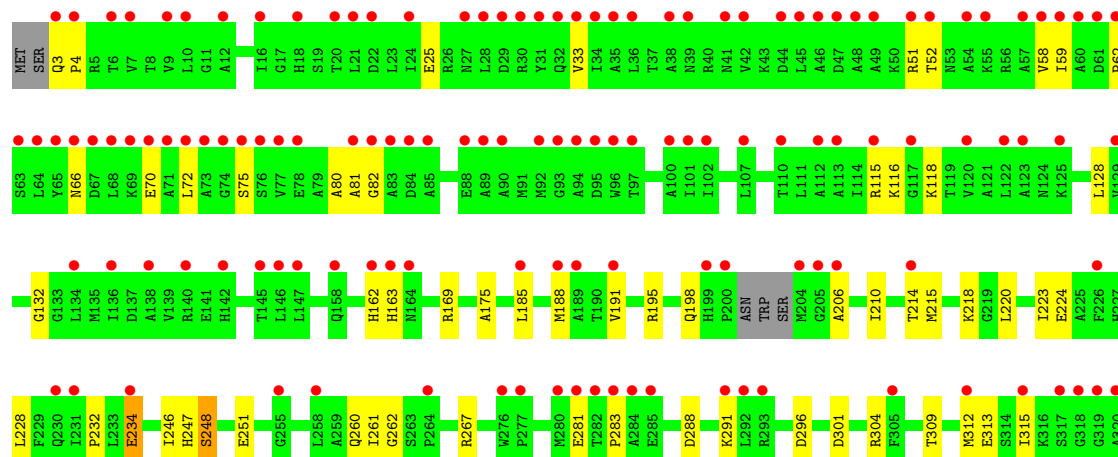
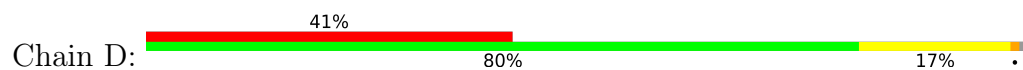


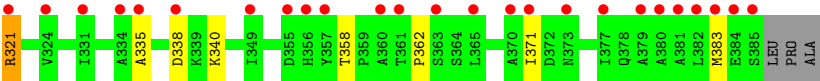


• Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase



• Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.70Å 93.20Å 98.60Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	29.63 – 1.91 29.63 – 1.91	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.63-1.91) 96.2 (29.63-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.230 0.295 , 0.316	Depositor DCC
R_{free} test set	2812 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12721	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0945e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT

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	0.35	0/2915	0.86	4/3953 (0.1%)
1	B	0.37	0/2934	0.86	6/3978 (0.2%)
1	C	0.35	0/2906	0.87	2/3940 (0.1%)
1	D	0.35	0/2920	0.85	1/3959 (0.0%)
All	All	0.36	0/11675	0.86	13/15830 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	246	ILE	N-CA-C	-5.84	99.89	108.54
1	D	246	ILE	N-CA-C	-5.77	100.00	108.54
1	A	31	TYR	N-CA-C	5.76	118.60	109.50
1	A	246	ILE	N-CA-C	-5.75	100.03	108.54
1	B	246	ILE	N-CA-C	-5.71	99.49	108.23
1	B	122	LEU	N-CA-C	5.29	117.35	108.73
1	B	151	SER	N-CA-C	5.10	119.78	111.37
1	C	122	LEU	N-CA-C	5.09	117.05	108.96
1	B	26	ARG	N-CA-C	-5.07	106.87	113.16
1	B	149	VAL	N-CA-C	5.07	116.95	111.58
1	A	241	HIS	CA-C-N	5.03	126.13	119.84
1	A	241	HIS	C-N-CA	5.03	126.13	119.84
1	B	230	GLN	N-CA-C	5.01	118.35	111.54

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	2867	0	2903	37	0
1	B	2885	0	2919	36	0
1	C	2858	0	2895	46	0
1	D	2871	0	2903	49	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	1	0
2	D	4	0	3	0	0
3	A	297	0	0	2	0
3	B	349	0	0	2	1
3	C	291	0	0	4	1
3	D	287	0	0	5	0
All	All	12721	0	11632	165	1

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 7.

All (165) 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:362:PRO:HG3	1:A:371:ILE:HD12	1.63	0.81
1:C:362:PRO:HG3	1:C:371:ILE:HD12	1.63	0.80
1:D:234:GLU:H	1:D:234:GLU:CD	1.92	0.77
1:B:234:GLU:H	1:B:234:GLU:CD	1.93	0.76
1:D:66:ASN:O	1:D:70:GLU:HG3	1.87	0.73
1:A:234:GLU:CD	1:A:234:GLU:H	1.97	0.71
1:C:301:ASP:OD2	1:C:304:ARG:HD3	1.90	0.70
1:B:267:ARG:CZ	1:B:283:PRO:HG2	2.22	0.69
1:C:234:GLU:H	1:C:234:GLU:CD	1.99	0.69
1:C:321:ARG:HB2	1:C:322:PRO:HD3	1.75	0.68
1:D:3:GLN:HB3	1:D:4:PRO:HA	1.75	0.68
1:D:185:LEU:HD23	1:D:188:MET:HE3	1.77	0.67
1:A:321:ARG:HB2	1:A:322:PRO:HD3	1.77	0.67
1:D:321:ARG:HG2	1:D:321:ARG:HH11	1.61	0.66
1:C:233:LEU:HD13	1:C:312:MET:HE1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LEU:HD12	1:A:387:PRO:HD2	1.78	0.66
1:C:267:ARG:CZ	1:C:283:PRO:HG2	2.25	0.65
1:A:233:LEU:HD13	1:A:312:MET:HE1	1.81	0.63
1:D:267:ARG:CZ	1:D:283:PRO:HG2	2.29	0.63
1:B:199:HIS:HE2	1:B:203:SER:N	1.96	0.62
1:C:293:ARG:HG2	1:C:294:GLN:HG3	1.81	0.62
1:D:335:ALA:HB2	1:D:383:MET:HE2	1.81	0.62
1:B:362:PRO:HG3	1:B:371:ILE:HD12	1.80	0.62
1:B:362:PRO:HG3	1:B:371:ILE:CD1	2.32	0.60
1:B:43:LYS:HE2	1:B:47:ASP:OD2	2.02	0.60
1:B:386:LEU:O	1:B:386:LEU:HD23	2.03	0.59
1:C:208:ILE:HG12	3:C:1559:HOH:O	2.02	0.58
1:A:301:ASP:OD2	1:A:304:ARG:HD3	2.01	0.58
1:D:301:ASP:OD2	1:D:304:ARG:HD3	2.04	0.58
1:D:312:MET:HE1	3:D:1552:HOH:O	2.04	0.58
1:C:309:THR:O	1:C:313:GLU:HG3	2.03	0.57
1:D:288:ASP:CG	1:D:291:LYS:HG2	2.30	0.57
1:B:267:ARG:NH1	1:B:283:PRO:HG2	2.19	0.57
1:D:321:ARG:HH21	1:D:358:THR:HG21	1.69	0.56
1:C:380:ALA:O	1:C:384:GLU:HG2	2.05	0.56
1:A:65:TYR:CZ	1:A:69:LYS:HD2	2.41	0.55
1:A:309:THR:O	1:A:313:GLU:HG3	2.06	0.55
1:D:25:GLU:OE1	1:D:51:ARG:HD3	2.06	0.55
1:D:116:LYS:HG3	3:D:1355:HOH:O	2.07	0.55
1:D:321:ARG:HH21	1:D:358:THR:CG2	2.19	0.55
1:B:47:ASP:O	1:B:51:ARG:HG3	2.07	0.54
1:D:188:MET:HA	1:D:191:VAL:HG23	1.90	0.54
1:A:267:ARG:CZ	1:A:283:PRO:HG2	2.38	0.54
1:D:72:LEU:O	1:D:75:SER:HB3	2.09	0.53
1:D:362:PRO:HG3	1:D:371:ILE:HD12	1.91	0.53
1:B:203:SER:O	1:B:204:MET:O	2.27	0.52
1:A:72:LEU:O	1:A:75:SER:HB3	2.08	0.52
1:D:309:THR:O	1:D:313:GLU:HG3	2.10	0.52
1:A:226:PHE:CD2	1:A:315:ILE:HD11	2.45	0.52
1:D:267:ARG:NH1	1:D:283:PRO:HG2	2.25	0.52
1:D:128:LEU:HD13	1:D:228:LEU:HG	1.92	0.51
1:A:162:HIS:O	1:A:163:HIS:HB2	2.11	0.51
1:A:312:MET:O	1:A:312:MET:HE3	2.10	0.51
1:C:128:LEU:HD13	1:C:228:LEU:HG	1.92	0.51
1:D:232:PRO:HB3	1:D:234:GLU:OE2	2.10	0.51
1:D:321:ARG:HE	1:D:358:THR:HG22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ASP:OD2	1:B:304:ARG:HD3	2.11	0.50
1:C:188:MET:O	1:C:191:VAL:HG22	2.11	0.50
1:A:188:MET:O	1:A:191:VAL:HG22	2.12	0.50
1:B:7:VAL:HG12	1:B:96:TRP:HB3	1.93	0.50
1:D:198:GLN:OE1	1:D:198:GLN:HA	2.11	0.50
1:C:193:PRO:HD2	1:C:194:GLU:OE2	2.11	0.49
1:A:208:ILE:HG12	3:A:1383:HOH:O	2.11	0.49
1:C:233:LEU:HD13	1:C:312:MET:CE	2.41	0.49
1:D:185:LEU:HA	1:D:188:MET:HE3	1.95	0.49
1:C:272:HIS:HB2	3:D:1469:HOH:O	2.13	0.48
1:D:362:PRO:HG3	1:D:371:ILE:CD1	2.42	0.48
1:D:185:LEU:HD23	1:D:188:MET:CE	2.43	0.48
1:B:234:GLU:CD	1:B:234:GLU:N	2.68	0.48
1:D:220:LEU:O	1:D:224:GLU:HG3	2.12	0.48
1:D:223:ILE:HA	1:D:315:ILE:HD11	1.94	0.48
1:B:335:ALA:HB2	1:B:383:MET:HE2	1.95	0.48
1:D:338:ASP:OD1	1:D:340:LYS:HE3	2.13	0.48
1:A:65:TYR:CE2	1:A:69:LYS:HD2	2.48	0.48
1:A:214:THR:O	1:A:215:MET:HB2	2.13	0.48
1:C:214:THR:O	1:C:215:MET:HB2	2.14	0.47
1:A:194:GLU:O	1:A:198:GLN:HB2	2.14	0.47
1:C:312:MET:O	1:C:312:MET:HE3	2.14	0.47
1:A:362:PRO:HG3	1:A:371:ILE:CD1	2.36	0.47
1:C:320:ALA:HB1	1:C:371:ILE:HD13	1.96	0.47
1:A:33:VAL:HG21	1:A:52:THR:HB	1.97	0.47
1:C:72:LEU:HD12	1:C:79:ALA:HB2	1.97	0.47
1:C:91:MET:HE3	3:C:1355:HOH:O	2.15	0.47
1:D:206:ALA:O	1:D:210:ILE:HG12	2.15	0.47
1:D:59:ILE:O	1:D:81:ALA:HA	2.15	0.46
1:D:118:LYS:HE3	3:D:1457:HOH:O	2.15	0.46
1:B:62:PRO:HG3	1:B:82:GLY:HA2	1.97	0.46
1:C:253:LEU:HD13	1:D:281:GLU:HG2	1.97	0.46
1:B:162:HIS:O	1:B:163:HIS:HB2	2.15	0.46
1:C:162:HIS:O	1:C:163:HIS:HB2	2.16	0.46
1:C:226:PHE:CD2	1:C:315:ILE:HD11	2.51	0.46
1:A:233:LEU:HD13	1:A:312:MET:CE	2.44	0.45
1:B:214:THR:O	1:B:215:MET:HB2	2.15	0.45
1:D:33:VAL:HG21	1:D:52:THR:HB	1.98	0.45
1:D:214:THR:O	1:D:215:MET:HB2	2.16	0.45
1:C:169:ARG:HD2	1:C:251:GLU:OE2	2.16	0.45
1:D:169:ARG:HD2	1:D:251:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:SER:HB2	3:B:1422:HOH:O	2.17	0.45
1:C:294:GLN:HG2	1:D:296:ASP:OD1	2.17	0.45
1:C:321:ARG:CB	1:C:322:PRO:HD3	2.45	0.45
1:B:267:ARG:NH1	1:B:283:PRO:CG	2.79	0.45
1:C:251:GLU:HG3	1:C:257:ILE:HG12	1.99	0.44
1:C:66:ASN:O	1:C:70:GLU:HG3	2.17	0.44
1:A:92:MET:HE3	3:A:1567:HOH:O	2.17	0.44
1:A:181:ARG:C	1:A:304:ARG:HH22	2.26	0.44
1:B:223:ILE:HG12	1:B:315:ILE:CG1	2.48	0.44
1:A:251:GLU:HG3	1:A:257:ILE:HG12	1.99	0.44
1:D:321:ARG:HG2	1:D:321:ARG:NH1	2.30	0.44
1:C:316:LYS:HD2	3:C:1564:HOH:O	2.18	0.44
1:B:199:HIS:HB3	3:B:1577:HOH:O	2.17	0.44
1:D:3:GLN:HA	1:D:4:PRO:C	2.43	0.44
1:A:234:GLU:CD	1:A:234:GLU:N	2.73	0.43
1:C:267:ARG:NH1	1:C:283:PRO:HG2	2.34	0.43
1:D:115:ARG:HD2	3:D:1522:HOH:O	2.18	0.43
1:B:203:SER:O	1:B:204:MET:C	2.62	0.43
1:C:128:LEU:HA	1:C:132:GLY:HA2	2.00	0.43
1:D:162:HIS:O	1:D:163:HIS:HB2	2.18	0.43
1:D:175:ALA:HA	1:D:218:LYS:HE3	2.01	0.43
1:C:175:ALA:CB	1:C:218:LYS:HE3	2.49	0.43
1:C:292:LEU:O	1:C:293:ARG:HB3	2.18	0.43
1:D:58:VAL:HG22	1:D:80:ALA:HB3	2.00	0.43
1:A:223:ILE:HG12	1:A:315:ILE:HB	2.01	0.43
1:D:128:LEU:HA	1:D:132:GLY:HA2	2.01	0.43
1:D:234:GLU:CD	1:D:234:GLU:N	2.70	0.43
1:B:39:ASN:HA	1:B:60:ALA:HB3	2.01	0.43
1:B:128:LEU:HD13	1:B:228:LEU:HG	2.01	0.42
1:A:128:LEU:HD13	1:A:228:LEU:HG	2.00	0.42
1:B:275:ALA:O	1:B:276:TRP:C	2.63	0.42
1:C:39:ASN:HB3	2:C:1303:ACT:C	2.50	0.42
1:B:3:GLN:HG2	1:B:4:PRO:HD2	2.01	0.42
1:C:218:LYS:HA	1:C:218:LYS:HD3	1.81	0.42
1:D:62:PRO:HG3	1:D:82:GLY:HA2	2.00	0.42
1:C:193:PRO:O	1:C:197:VAL:HG22	2.19	0.42
1:C:59:ILE:O	1:C:81:ALA:HA	2.19	0.42
1:C:153:HIS:CE1	1:C:224:GLU:HB2	2.55	0.42
1:B:175:ALA:HA	1:B:218:LYS:HE3	2.02	0.42
1:D:261:ILE:HG22	1:D:262:GLY:N	2.35	0.42
1:C:234:GLU:CD	1:C:234:GLU:N	2.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:THR:HG22	3:C:1435:HOH:O	2.19	0.42
1:B:207:LYS:NZ	1:B:211:ASP:OD2	2.50	0.41
1:D:247:HIS:O	1:D:248:SER:CB	2.68	0.41
1:A:223:ILE:HG23	1:A:315:ILE:HD13	2.02	0.41
1:B:59:ILE:O	1:B:59:ILE:HG23	2.19	0.41
1:B:310:LEU:HD21	1:B:351:GLU:HG3	2.01	0.41
1:B:366:GLU:N	1:B:366:GLU:CD	2.78	0.41
1:D:3:GLN:HB3	1:D:4:PRO:CA	2.45	0.41
1:B:188:MET:HA	1:B:191:VAL:HG23	2.03	0.41
1:B:223:ILE:HA	1:B:315:ILE:HD11	2.03	0.41
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.96	0.41
1:A:218:LYS:HA	1:A:218:LYS:HD3	1.82	0.41
1:A:321:ARG:CB	1:A:322:PRO:HD3	2.49	0.41
1:B:349:ILE:HD12	1:B:383:MET:HA	2.03	0.41
1:C:232:PRO:HB3	1:C:234:GLU:OE2	2.20	0.41
1:C:247:HIS:O	1:C:248:SER:CB	2.68	0.41
1:A:247:HIS:O	1:A:248:SER:CB	2.68	0.41
1:A:268:THR:HB	1:A:269:PRO:CD	2.51	0.41
1:A:361:THR:HA	1:A:362:PRO:HD3	1.89	0.41
1:A:374:GLU:O	1:A:378:GLN:HG2	2.21	0.41
1:B:247:HIS:O	1:B:248:SER:CB	2.69	0.40
1:A:293:ARG:HG2	1:A:294:GLN:HG3	2.02	0.40
1:C:170:ARG:NE	1:C:251:GLU:OE1	2.46	0.40
1:C:374:GLU:O	1:C:378:GLN:HG2	2.21	0.40
1:C:365:LEU:HD23	1:C:365:LEU:HA	1.93	0.40
1:A:281:GLU:HG2	1:B:253:LEU:HB3	2.03	0.40
1:C:233:LEU:HB3	1:C:312:MET:HE1	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1567:HOH:O	3:C:1473:HOH:O[2_655]	2.07	0.13

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	376/388 (97%)	367 (98%)	8 (2%)	1 (0%)	36	26
1	B	378/388 (97%)	367 (97%)	9 (2%)	2 (0%)	24	14
1	C	375/388 (97%)	360 (96%)	13 (4%)	2 (0%)	24	14
1	D	376/388 (97%)	367 (98%)	8 (2%)	1 (0%)	36	26
All	All	1505/1552 (97%)	1461 (97%)	38 (2%)	6 (0%)	30	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	MET
1	A	248	SER
1	B	248	SER
1	C	248	SER
1	D	248	SER
1	C	387	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	301/308 (98%)	299 (99%)	2 (1%)	76	73
1	B	303/308 (98%)	300 (99%)	3 (1%)	68	64
1	C	299/308 (97%)	295 (99%)	4 (1%)	61	53
1	D	301/308 (98%)	297 (99%)	4 (1%)	61	53
All	All	1204/1232 (98%)	1191 (99%)	13 (1%)	65	60

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	GLU
1	A	260	GLN
1	B	195	ARG
1	B	234	GLU
1	B	260	GLN
1	C	194	GLU
1	C	234	GLU
1	C	260	GLN
1	C	316	LYS
1	D	195	ARG
1	D	234	GLU
1	D	260	GLN
1	D	321	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	39	ASN
1	A	53	ASN
1	A	162	HIS
1	A	164	ASN
1	A	198	GLN
1	A	260	GLN
1	B	32	GLN
1	B	39	ASN
1	B	53	ASN
1	B	142	HIS
1	B	227	HIS
1	B	260	GLN
1	B	329	ASN
1	C	53	ASN
1	C	164	ASN
1	C	260	GLN
1	D	39	ASN
1	D	53	ASN
1	D	142	HIS
1	D	260	GLN
1	D	373	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	ACT	A	1301	-	3,3,3	1.26	1 (33%)	3,3,3	0.72	0
2	ACT	D	1304	-	3,3,3	1.22	0	3,3,3	0.70	0
2	ACT	C	1303	-	3,3,3	1.27	1 (33%)	3,3,3	0.71	0
2	ACT	B	1302	-	3,3,3	1.22	0	3,3,3	0.71	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1303	ACT	O-C	2.11	1.31	1.22
2	A	1301	ACT	O-C	2.07	1.31	1.22

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1303	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	380/388 (97%)	2.77	294 (77%) 0 0	8, 18, 33, 53	0
1	B	382/388 (98%)	1.94	167 (43%) 0 0	9, 17, 34, 57	0
1	C	379/388 (97%)	2.04	179 (47%) 0 0	10, 18, 33, 56	0
1	D	380/388 (97%)	1.92	159 (41%) 0 0	10, 19, 34, 62	0
All	All	1521/1552 (98%)	2.17	799 (52%) 0 0	8, 18, 33, 62	0

All (799) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	386	LEU	8.6
1	C	386	LEU	5.6
1	A	357	TYR	5.5
1	A	386	LEU	5.4
1	A	77	VAL	5.2
1	C	29	ASP	5.2
1	D	3	GLN	5.1
1	A	49	ALA	5.1
1	D	318	GLY	4.9
1	C	388	ALA	4.9
1	A	65	TYR	4.9
1	A	69	LYS	4.9
1	A	81	ALA	4.8
1	C	30	ARG	4.7
1	A	197	VAL	4.7
1	D	163	HIS	4.7
1	A	315	ILE	4.7
1	A	369	PHE	4.6
1	A	64	LEU	4.6
1	D	71	ALA	4.5
1	D	4	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	198	GLN	4.5
1	A	359	PRO	4.4
1	C	387	PRO	4.4
1	A	2	SER	4.4
1	A	71	ALA	4.4
1	A	206	ALA	4.4
1	A	58	VAL	4.4
1	D	383	MET	4.4
1	D	277	PRO	4.4
1	C	356	HIS	4.4
1	A	213	ALA	4.3
1	C	363	SER	4.3
1	A	387	PRO	4.3
1	A	358	THR	4.3
1	A	196	ALA	4.3
1	C	87	VAL	4.3
1	C	61	ASP	4.3
1	C	365	LEU	4.2
1	A	230	GLN	4.2
1	B	3	GLN	4.2
1	A	210	ILE	4.2
1	C	65	TYR	4.2
1	A	339	LYS	4.2
1	A	24	ILE	4.2
1	B	200	PRO	4.2
1	A	46	ALA	4.1
1	A	189	ALA	4.1
1	A	335	ALA	4.1
1	A	54	ALA	4.1
1	C	72	LEU	4.1
1	A	336	PHE	4.1
1	A	349	ILE	4.1
1	A	20	THR	4.1
1	A	209	SER	4.1
1	A	35	ALA	4.0
1	D	73	ALA	4.0
1	C	318	GLY	4.0
1	A	48	ALA	4.0
1	D	75	SER	4.0
1	C	78	GLU	4.0
1	A	75	SER	4.0
1	A	42	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	102	ILE	4.0
1	A	377	ILE	4.0
1	D	315	ILE	4.0
1	D	356	HIS	3.9
1	D	384	GLU	3.9
1	A	86	LEU	3.9
1	A	12	ALA	3.9
1	A	236	PHE	3.9
1	D	74	GLY	3.9
1	B	356	HIS	3.9
1	B	167	TYR	3.9
1	A	72	LEU	3.9
1	A	290	THR	3.9
1	B	70	GLU	3.9
1	B	383	MET	3.9
1	B	256	SER	3.9
1	A	38	ALA	3.9
1	D	72	LEU	3.8
1	A	51	ARG	3.8
1	A	101	ILE	3.8
1	A	378	GLN	3.8
1	B	233	LEU	3.8
1	A	328	ALA	3.8
1	C	131	ALA	3.8
1	A	208	ILE	3.8
1	A	226	PHE	3.8
1	A	184	SER	3.8
1	C	357	TYR	3.8
1	A	112	ALA	3.8
1	C	320	ALA	3.8
1	D	385	SER	3.8
1	A	322	PRO	3.7
1	A	45	LEU	3.7
1	A	30	ARG	3.7
1	C	102	ILE	3.7
1	C	369	PHE	3.7
1	A	205	GLY	3.7
1	B	69	LYS	3.7
1	A	76	SER	3.7
1	A	129	VAL	3.7
1	A	53	ASN	3.7
1	A	62	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	362	PRO	3.7
1	C	68	LEU	3.7
1	A	104	CYS	3.7
1	A	371	ILE	3.7
1	A	27	ASN	3.7
1	A	310	LEU	3.6
1	A	360	ALA	3.6
1	B	73	ALA	3.6
1	A	11	GLY	3.6
1	A	103	GLY	3.6
1	C	197	VAL	3.6
1	B	303	GLU	3.6
1	C	75	SER	3.6
1	D	360	ALA	3.6
1	B	77	VAL	3.6
1	D	70	GLU	3.6
1	C	63	SER	3.6
1	A	73	ALA	3.6
1	A	91	MET	3.6
1	B	312	MET	3.6
1	C	18	HIS	3.6
1	A	66	ASN	3.5
1	B	255	GLY	3.5
1	A	244	SER	3.5
1	A	321	ARG	3.5
1	A	245	VAL	3.5
1	A	292	LEU	3.5
1	D	284	ALA	3.5
1	A	342	GLY	3.5
1	B	318	GLY	3.5
1	A	385	SER	3.5
1	A	87	VAL	3.5
1	A	240	VAL	3.5
1	B	168	VAL	3.5
1	A	375	ALA	3.5
1	D	28	LEU	3.5
1	A	33	VAL	3.4
1	A	74	GLY	3.4
1	A	157	PHE	3.4
1	D	382	LEU	3.4
1	C	364	SER	3.4
1	C	66	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	66	ASN	3.4
1	A	316	LYS	3.4
1	A	149	VAL	3.4
1	A	354	LEU	3.4
1	D	63	SER	3.4
1	D	65	TYR	3.4
1	D	162	HIS	3.4
1	A	132	GLY	3.4
1	A	318	GLY	3.4
1	B	381	ALA	3.4
1	C	140	ARG	3.4
1	A	282	THR	3.4
1	D	199	HIS	3.3
1	B	231	ILE	3.3
1	A	80	ALA	3.3
1	A	89	ALA	3.3
1	A	332	ALA	3.3
1	C	81	ALA	3.3
1	A	365	LEU	3.3
1	B	185	LEU	3.3
1	D	64	LEU	3.3
1	A	229	PHE	3.3
1	A	183	THR	3.3
1	B	44	ASP	3.3
1	B	355	ASP	3.3
1	A	127	SER	3.3
1	C	77	VAL	3.3
1	B	72	LEU	3.3
1	D	185	LEU	3.3
1	A	37	THR	3.3
1	D	276	TRP	3.3
1	A	39	ASN	3.3
1	A	261	ILE	3.3
1	C	377	ILE	3.3
1	B	129	VAL	3.3
1	D	57	ALA	3.3
1	D	94	ALA	3.3
1	D	113	ALA	3.3
1	D	381	ALA	3.3
1	A	13	THR	3.3
1	A	233	LEU	3.3
1	A	382	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	47	ASP	3.3
1	A	297	PHE	3.3
1	B	180	PHE	3.3
1	A	41	ASN	3.3
1	A	373	ASN	3.3
1	B	349	ILE	3.2
1	A	307	ALA	3.2
1	D	85	ALA	3.2
1	A	44	ASP	3.2
1	A	67	ASP	3.2
1	A	23	LEU	3.2
1	A	28	LEU	3.2
1	C	359	PRO	3.2
1	D	69	LYS	3.2
1	A	18	HIS	3.2
1	C	73	ALA	3.2
1	C	85	ALA	3.2
1	A	52	THR	3.2
1	B	183	THR	3.2
1	D	52	THR	3.2
1	A	264	PRO	3.2
1	A	306	PRO	3.2
1	A	308	LEU	3.2
1	A	78	GLU	3.2
1	A	17	GLY	3.2
1	B	160	PHE	3.2
1	B	343	PHE	3.2
1	B	199	HIS	3.2
1	A	34	ILE	3.2
1	A	60	ALA	3.2
1	A	347	ALA	3.2
1	B	302	TYR	3.2
1	D	48	ALA	3.2
1	A	8	THR	3.2
1	A	190	THR	3.2
1	A	309	THR	3.2
1	A	350	VAL	3.2
1	A	55	LYS	3.2
1	D	21	LEU	3.2
1	C	385	SER	3.2
1	A	160	PHE	3.2
1	C	163	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	140	ARG	3.2
1	C	355	ASP	3.2
1	D	44	ASP	3.2
1	A	284	ALA	3.1
1	A	340	LYS	3.1
1	A	22	ASP	3.1
1	A	29	ASP	3.1
1	A	370	ALA	3.1
1	A	270	ILE	3.1
1	C	232	PRO	3.1
1	B	203	SER	3.1
1	D	34	ILE	3.1
1	B	342	GLY	3.1
1	B	354	LEU	3.1
1	D	204	MET	3.1
1	C	144	THR	3.1
1	C	277	PRO	3.1
1	A	219	GLY	3.1
1	A	231	ILE	3.1
1	A	302	TYR	3.1
1	A	47	ASP	3.1
1	B	305	PHE	3.1
1	A	6	THR	3.1
1	D	76	SER	3.1
1	A	14	GLY	3.1
1	A	57	ALA	3.1
1	A	100	ALA	3.1
1	B	225	ALA	3.1
1	B	299	ALA	3.1
1	C	360	ALA	3.1
1	B	371	ILE	3.0
1	C	231	ILE	3.0
1	A	63	SER	3.0
1	B	362	PRO	3.0
1	A	216	MET	3.0
1	A	15	SER	3.0
1	A	180	PHE	3.0
1	A	263	SER	3.0
1	C	127	SER	3.0
1	D	363	SER	3.0
1	A	113	ALA	3.0
1	A	380	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	381	ALA	3.0
1	C	49	ALA	3.0
1	C	370	ALA	3.0
1	B	341	ILE	3.0
1	A	222	LEU	3.0
1	B	384	GLU	3.0
1	C	7	VAL	3.0
1	A	241	HIS	3.0
1	A	305	PHE	3.0
1	C	148	PRO	3.0
1	A	79	ALA	3.0
1	A	186	ALA	3.0
1	B	360	ALA	3.0
1	C	315	ILE	3.0
1	C	371	ILE	3.0
1	A	163	HIS	2.9
1	C	45	LEU	2.9
1	C	86	LEU	2.9
1	A	317	SER	2.9
1	B	385	SER	2.9
1	D	357	TYR	2.9
1	D	51	ARG	2.9
1	A	82	GLY	2.9
1	D	117	GLY	2.9
1	A	70	GLU	2.9
1	A	275	ALA	2.9
1	C	123	ALA	2.9
1	C	138	ALA	2.9
1	A	36	LEU	2.9
1	A	68	LEU	2.9
1	A	111	LEU	2.9
1	A	287	LEU	2.9
1	A	344	LEU	2.9
1	D	7	VAL	2.9
1	A	280	MET	2.9
1	B	143	GLY	2.9
1	A	193	PRO	2.9
1	A	362	PRO	2.9
1	C	226	PHE	2.9
1	C	71	ALA	2.9
1	A	355	ASP	2.9
1	A	21	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	253	LEU	2.9
1	D	68	LEU	2.9
1	D	107	LEU	2.9
1	C	141	GLU	2.9
1	A	93	GLY	2.9
1	A	119	THR	2.9
1	C	41	ASN	2.9
1	B	306	PRO	2.9
1	D	200	PRO	2.9
1	B	297	PHE	2.9
1	B	369	PHE	2.9
1	B	370	ALA	2.9
1	C	109	ALA	2.9
1	D	206	ALA	2.9
1	C	151	SER	2.9
1	B	315	ILE	2.9
1	C	64	LEU	2.9
1	C	111	LEU	2.9
1	C	208	ILE	2.9
1	B	205	GLY	2.9
1	B	271	GLY	2.9
1	C	74	GLY	2.9
1	A	120	VAL	2.8
1	D	33	VAL	2.8
1	A	161	PRO	2.8
1	A	85	ALA	2.8
1	B	71	ALA	2.8
1	C	380	ALA	2.8
1	A	61	ASP	2.8
1	C	366	GLU	2.8
1	B	317	SER	2.8
1	A	266	MET	2.8
1	A	383	MET	2.8
1	A	16	ILE	2.8
1	B	128	LEU	2.8
1	C	28	LEU	2.8
1	C	134	LEU	2.8
1	D	164	ASN	2.8
1	C	129	VAL	2.8
1	A	291	LYS	2.8
1	C	322	PRO	2.8
1	B	65	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	265	ASP	2.8
1	A	105	ALA	2.8
1	A	334	ALA	2.8
1	C	186	ALA	2.8
1	D	138	ALA	2.8
1	D	317	SER	2.8
1	A	217	ASN	2.8
1	D	41	ASN	2.8
1	C	205	GLY	2.8
1	C	122	LEU	2.8
1	C	185	LEU	2.8
1	C	233	LEU	2.8
1	C	378	GLN	2.8
1	A	192	THR	2.8
1	B	163	HIS	2.8
1	C	349	ILE	2.8
1	D	24	ILE	2.8
1	B	42	VAL	2.8
1	C	67	ASP	2.8
1	A	94	ALA	2.8
1	D	100	ALA	2.8
1	B	236	PHE	2.8
1	A	43	LYS	2.8
1	A	97	THR	2.8
1	B	228	LEU	2.8
1	D	134	LEU	2.8
1	A	191	VAL	2.8
1	C	317	SER	2.7
1	B	357	TYR	2.7
1	A	26	ARG	2.7
1	A	323	ALA	2.7
1	B	155	ALA	2.7
1	C	48	ALA	2.7
1	C	228	LEU	2.7
1	A	59	ILE	2.7
1	C	136	ILE	2.7
1	C	367	ASP	2.7
1	D	59	ILE	2.7
1	D	84	ASP	2.7
1	B	30	ARG	2.7
1	C	149	VAL	2.7
1	A	109	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	70	GLU	2.7
1	C	83	ALA	2.7
1	D	90	ALA	2.7
1	A	227	HIS	2.7
1	B	309	THR	2.7
1	C	92	MET	2.7
1	C	21	LEU	2.7
1	A	4	PRO	2.7
1	A	179	PRO	2.7
1	B	359	PRO	2.7
1	A	341	ILE	2.7
1	D	101	ILE	2.7
1	B	198	GLN	2.7
1	D	30	ARG	2.7
1	B	164	ASN	2.7
1	C	50	LYS	2.7
1	D	78	GLU	2.7
1	A	96	TRP	2.7
1	A	138	ALA	2.7
1	C	275	ALA	2.7
1	D	54	ALA	2.7
1	A	143	GLY	2.7
1	D	319	GLY	2.7
1	A	185	LEU	2.7
1	A	269	PRO	2.7
1	B	63	SER	2.7
1	B	161	PRO	2.7
1	C	382	LEU	2.7
1	D	258	LEU	2.7
1	A	50	LYS	2.7
1	C	43	LYS	2.7
1	D	55	LYS	2.7
1	C	120	VAL	2.7
1	D	58	VAL	2.7
1	D	320	ALA	2.6
1	B	204	MET	2.6
1	B	254	ASP	2.6
1	D	226	PHE	2.6
1	A	351	GLU	2.6
1	C	384	GLU	2.6
1	C	314	SER	2.6
1	B	4	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	239	LEU	2.6
1	B	68	LEU	2.6
1	D	39	ASN	2.6
1	C	270	ILE	2.6
1	A	92	MET	2.6
1	A	333	VAL	2.6
1	C	319	GLY	2.6
1	D	129	VAL	2.6
1	A	83	ALA	2.6
1	A	123	ALA	2.6
1	A	345	ASP	2.6
1	B	284	ALA	2.6
1	B	293	ARG	2.6
1	C	44	ASP	2.6
1	C	60	ALA	2.6
1	C	84	ASP	2.6
1	D	29	ASP	2.6
1	D	380	ALA	2.6
1	B	252	TYR	2.6
1	A	145	THR	2.6
1	D	146	LEU	2.6
1	B	216	MET	2.6
1	A	117	GLY	2.6
1	C	106	GLY	2.6
1	D	22	ASP	2.6
1	A	168	VAL	2.6
1	B	375	ALA	2.6
1	B	55	LYS	2.6
1	A	214	THR	2.6
1	B	66	ASN	2.6
1	C	373	ASN	2.6
1	A	356	HIS	2.6
1	D	283	PRO	2.6
1	A	289	PHE	2.6
1	A	128	LEU	2.6
1	A	312	MET	2.6
1	D	321	ARG	2.6
1	B	230	GLN	2.6
1	A	303	GLU	2.6
1	A	346	ILE	2.6
1	D	38	ALA	2.6
1	D	189	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	334	ALA	2.6
1	B	165	ARG	2.5
1	A	194	GLU	2.5
1	C	82	GLY	2.5
1	A	329	ASN	2.5
1	A	379	ALA	2.5
1	B	79	ALA	2.5
1	B	379	ALA	2.5
1	C	94	ALA	2.5
1	A	139	VAL	2.5
1	B	324	VAL	2.5
1	B	350	VAL	2.5
1	A	273	THR	2.5
1	D	6	THR	2.5
1	C	230	GLN	2.5
1	D	32	GLN	2.5
1	C	104	CYS	2.5
1	C	166	ASP	2.5
1	D	31	TYR	2.5
1	A	343	PHE	2.5
1	B	352	LYS	2.5
1	C	146	LEU	2.5
1	D	205	GLY	2.5
1	D	349	ILE	2.5
1	B	321	ARG	2.5
1	A	99	ALA	2.5
1	A	131	ALA	2.5
1	A	320	ALA	2.5
1	C	206	ALA	2.5
1	A	313	GLU	2.5
1	A	353	THR	2.5
1	D	230	GLN	2.5
1	A	374	GLU	2.5
1	B	316	LYS	2.5
1	D	291	LYS	2.5
1	A	274	LEU	2.5
1	D	122	LEU	2.5
1	D	305	PHE	2.5
1	C	27	ASN	2.5
1	A	130	SER	2.5
1	A	172	ILE	2.5
1	A	223	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	208	ILE	2.5
1	B	210	ILE	2.5
1	B	257	ILE	2.5
1	B	346	ILE	2.5
1	D	136	ILE	2.5
1	B	186	ALA	2.5
1	B	311	ALA	2.5
1	B	347	ALA	2.5
1	C	57	ALA	2.5
1	C	99	ALA	2.5
1	C	112	ALA	2.5
1	C	110	THR	2.5
1	C	282	THR	2.5
1	A	7	VAL	2.5
1	A	9	VAL	2.5
1	A	324	VAL	2.5
1	D	42	VAL	2.5
1	D	67	ASP	2.5
1	C	4	PRO	2.5
1	A	115	ARG	2.4
1	A	195	ARG	2.4
1	D	93	GLY	2.4
1	A	220	LEU	2.4
1	B	157	PHE	2.4
1	C	23	LEU	2.4
1	D	371	ILE	2.4
1	D	60	ALA	2.4
1	A	40	ARG	2.4
1	A	25	GLU	2.4
1	D	18	HIS	2.4
1	B	382	LEU	2.4
1	C	31	TYR	2.4
1	C	76	SER	2.4
1	D	10	LEU	2.4
1	D	280	MET	2.4
1	D	125	LYS	2.4
1	A	238	ILE	2.4
1	B	301	ASP	2.4
1	C	137	ASP	2.4
1	D	355	ASP	2.4
1	C	290	THR	2.4
1	C	80	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	56	ARG	2.4
1	B	264	PRO	2.4
1	C	42	VAL	2.4
1	C	126	GLU	2.4
1	A	3	GLN	2.4
1	A	98	MET	2.4
1	A	314	SER	2.4
1	A	258	LEU	2.4
1	A	114	ILE	2.4
1	A	293	ARG	2.4
1	C	59	ILE	2.4
1	B	189	ALA	2.4
1	C	46	ALA	2.4
1	C	89	ALA	2.4
1	D	35	ALA	2.4
1	D	49	ALA	2.4
1	D	89	ALA	2.4
1	D	112	ALA	2.4
1	A	366	GLU	2.4
1	A	283	PRO	2.4
1	D	158	GLN	2.4
1	B	153	HIS	2.4
1	D	142	HIS	2.4
1	B	197	VAL	2.4
1	B	240	VAL	2.4
1	D	82	GLY	2.4
1	C	96	TRP	2.4
1	D	96	TRP	2.4
1	B	118	LYS	2.4
1	A	296	ASP	2.3
1	D	95	ASP	2.3
1	A	228	LEU	2.3
1	D	365	LEU	2.3
1	B	144	THR	2.3
1	B	361	THR	2.3
1	A	121	ALA	2.3
1	D	102	ILE	2.3
1	A	162	HIS	2.3
1	B	162	HIS	2.3
1	C	161	PRO	2.3
1	A	212	SER	2.3
1	B	9	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	209	SER	2.3
1	C	22	ASP	2.3
1	C	254	ASP	2.3
1	C	276	TRP	2.3
1	A	253	LEU	2.3
1	A	31	TYR	2.3
1	C	167	TYR	2.3
1	D	282	THR	2.3
1	A	326	ASN	2.3
1	C	164	ASN	2.3
1	D	123	ALA	2.3
1	B	171	ILE	2.3
1	C	114	ILE	2.3
1	C	177	GLY	2.3
1	A	286	SER	2.3
1	B	363	SER	2.3
1	D	293	ARG	2.3
1	A	187	GLU	2.3
1	C	194	GLU	2.3
1	C	351	GLU	2.3
1	C	10	LEU	2.3
1	C	107	LEU	2.3
1	A	268	THR	2.3
1	B	226	PHE	2.3
1	C	69	LYS	2.3
1	A	232	PRO	2.3
1	A	299	ALA	2.3
1	A	311	ALA	2.3
1	B	196	ALA	2.3
1	B	335	ALA	2.3
1	D	62	PRO	2.3
1	A	271	GLY	2.3
1	B	173	ILE	2.3
1	C	117	GLY	2.3
1	D	331	ILE	2.3
1	A	372	ASP	2.3
1	B	281	GLU	2.3
1	D	77	VAL	2.3
1	C	142	HIS	2.3
1	A	134	LEU	2.3
1	A	144	THR	2.3
1	A	325	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	292	LEU	2.3
1	B	344	LEU	2.3
1	C	135	MET	2.3
1	D	147	LEU	2.3
1	A	327	ALA	2.2
1	A	384	GLU	2.2
1	C	157	PHE	2.2
1	C	175	ALA	2.2
1	D	379	ALA	2.2
1	A	19	SER	2.2
1	A	84	ASP	2.2
1	A	136	ILE	2.2
1	D	231	ILE	2.2
1	D	324	VAL	2.2
1	A	154	ASN	2.2
1	B	227	HIS	2.2
1	A	215	MET	2.2
1	C	361	THR	2.2
1	B	21	LEU	2.2
1	B	166	ASP	2.2
1	B	176	SER	2.2
1	B	178	GLY	2.2
1	C	17	GLY	2.2
1	C	132	GLY	2.2
1	A	90	ALA	2.2
1	A	155	ALA	2.2
1	B	332	ALA	2.2
1	B	380	ALA	2.2
1	C	335	ALA	2.2
1	D	46	ALA	2.2
1	B	289	PHE	2.2
1	A	348	LYS	2.2
1	A	237	GLU	2.2
1	B	234	GLU	2.2
1	D	281	GLU	2.2
1	A	159	CYS	2.2
1	A	337	LEU	2.2
1	B	151	SER	2.2
1	B	248	SER	2.2
1	D	61	ASP	2.2
1	D	338	ASP	2.2
1	B	138	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	323	ALA	2.2
1	C	35	ALA	2.2
1	D	12	ALA	2.2
1	D	83	ALA	2.2
1	B	336	PHE	2.2
1	C	252	TYR	2.2
1	B	18	HIS	2.2
1	B	276	TRP	2.2
1	C	165	ARG	2.2
1	C	88	GLU	2.2
1	B	378	GLN	2.2
1	B	190	THR	2.2
1	D	361	THR	2.2
1	B	47	ASP	2.2
1	B	130	SER	2.2
1	B	74	GLY	2.2
1	B	287	LEU	2.2
1	C	354	LEU	2.2
1	D	370	ALA	2.2
1	A	165	ARG	2.2
1	D	188	MET	2.1
1	B	156	ILE	2.1
1	C	331	ILE	2.1
1	D	377	ILE	2.1
1	C	3	GLN	2.1
1	C	58	VAL	2.1
1	D	9	VAL	2.1
1	D	110	THR	2.1
1	D	214	THR	2.1
1	B	75	SER	2.1
1	C	244	SER	2.1
1	A	304	ARG	2.1
1	D	36	LEU	2.1
1	C	234	GLU	2.1
1	C	38	ALA	2.1
1	C	332	ALA	2.1
1	C	334	ALA	2.1
1	A	156	ILE	2.1
1	B	34	ILE	2.1
1	D	16	ILE	2.1
1	B	61	ASP	2.1
1	A	363	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	182	THR	2.1
1	B	214	THR	2.1
1	D	145	THR	2.1
1	A	250	VAL	2.1
1	B	304	ARG	2.1
1	B	333	VAL	2.1
1	B	368	VAL	2.1
1	D	285	GLU	2.1
1	C	383	MET	2.1
1	B	239	LEU	2.1
1	B	274	LEU	2.1
1	B	322	PRO	2.1
1	C	124	ASN	2.1
1	B	259	ALA	2.1
1	C	311	ALA	2.1
1	A	331	ILE	2.1
1	B	195	ARG	2.1
1	A	281	GLU	2.1
1	C	6	THR	2.1
1	D	97	THR	2.1
1	D	92	MET	2.1
1	B	250	VAL	2.1
1	C	139	VAL	2.1
1	D	27	ASN	2.1
1	D	120	VAL	2.1
1	A	146	LEU	2.1
1	C	36	LEU	2.1
1	D	292	LEU	2.1
1	C	379	ALA	2.1
1	D	81	ALA	2.1
1	D	335	ALA	2.1
1	C	195	ARG	2.1
1	C	16	ILE	2.0
1	C	156	ILE	2.0
1	D	88	GLU	2.0
1	D	312	MET	2.0
1	A	178	GLY	2.0
1	D	255	GLY	2.0
1	B	149	VAL	2.0
1	C	242	PRO	2.0
1	C	245	VAL	2.0
1	B	220	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	45	LEU	2.0
1	B	60	ALA	2.0
1	B	85	ALA	2.0
1	B	123	ALA	2.0
1	C	105	ALA	2.0
1	B	366	GLU	2.0
1	D	234	GLU	2.0
1	B	218	LYS	2.0
1	B	278	LYS	2.0
1	B	102	ILE	2.0
1	B	223	ILE	2.0
1	C	24	ILE	2.0
1	B	145	THR	2.0
1	C	103	GLY	2.0
1	D	20	THR	2.0
1	D	373	ASN	2.0
1	D	264	PRO	2.0
1	C	321	ARG	2.0
1	C	350	VAL	2.0
1	D	115	ARG	2.0
1	D	140	ARG	2.0
1	D	191	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	A	1301	4/4	0.56	0.22	29,30,30,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	B	1302	4/4	0.60	0.26	44,45,45,46	0
2	ACT	C	1303	4/4	0.63	0.17	34,35,36,36	0
2	ACT	D	1304	4/4	0.63	0.21	29,32,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.