Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 02:52 AM EST

PDB ID	:	1S3R
Title	:	Crystal structure of the human-specific toxin intermedilysin
Authors	:	Polekhina, G.; Giddings, K.S.; Tweten, R.K.; Parker, M.W.
Deposited on	:	2004-01-14
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 (i) 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 (i)) were used in the production of this report:

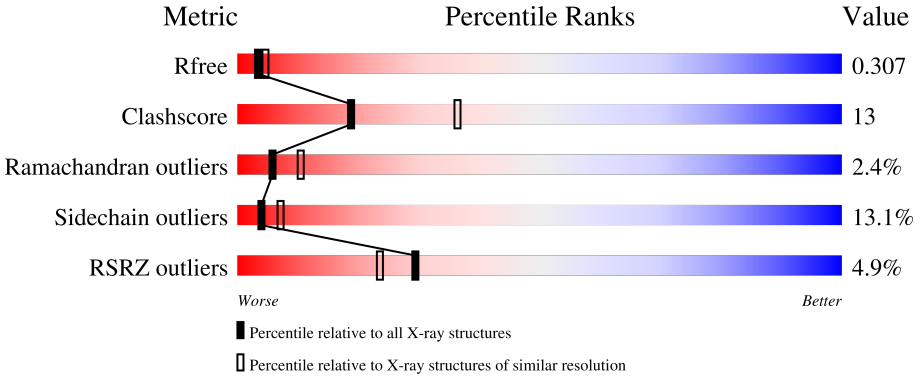
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	535	6%; 60%; 23%; • •; 12%
1	B	535	2%; 57%; 26%; 5% •; 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7827 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 intermedilysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	473	3678	2321	644	710	3	0	0	0
1	B	473	3678	2321	644	710	3	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP Q9LCB8
A	-1	GLY	-	expression tag	UNP Q9LCB8
A	0	GLY	-	expression tag	UNP Q9LCB8
A	1	SER	-	expression tag	UNP Q9LCB8
A	2	HIS	-	expression tag	UNP Q9LCB8
A	3	HIS	-	expression tag	UNP Q9LCB8
A	4	HIS	-	expression tag	UNP Q9LCB8
A	5	HIS	-	expression tag	UNP Q9LCB8
A	6	HIS	-	expression tag	UNP Q9LCB8
A	7	HIS	-	expression tag	UNP Q9LCB8
A	8	GLY	-	expression tag	UNP Q9LCB8
A	9	MET	-	expression tag	UNP Q9LCB8
A	10	ALA	-	expression tag	UNP Q9LCB8
A	11	SER	-	expression tag	UNP Q9LCB8
A	12	MET	-	expression tag	UNP Q9LCB8
A	13	THR	-	expression tag	UNP Q9LCB8
A	14	GLY	-	expression tag	UNP Q9LCB8
A	15	GLY	-	expression tag	UNP Q9LCB8
A	16	GLN	-	expression tag	UNP Q9LCB8
A	17	GLN	-	expression tag	UNP Q9LCB8
A	18	MET	-	expression tag	UNP Q9LCB8
A	19	GLY	-	expression tag	UNP Q9LCB8
A	20	ARG	-	expression tag	UNP Q9LCB8
A	21	ASP	-	expression tag	UNP Q9LCB8
A	22	LEU	-	expression tag	UNP Q9LCB8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	TYR	-	expression tag	UNP Q9LCB8
A	24	ASP	-	expression tag	UNP Q9LCB8
A	25	ASP	-	expression tag	UNP Q9LCB8
A	26	ASP	-	expression tag	UNP Q9LCB8
A	27	ASP	-	expression tag	UNP Q9LCB8
A	28	LYS	-	expression tag	UNP Q9LCB8
A	29	ASP	-	expression tag	UNP Q9LCB8
A	30	ARG	-	expression tag	UNP Q9LCB8
A	31	TRP	-	expression tag	UNP Q9LCB8
A	32	GLY	-	expression tag	UNP Q9LCB8
A	33	SER	-	expression tag	UNP Q9LCB8
B	-2	MET	-	expression tag	UNP Q9LCB8
B	-1	GLY	-	expression tag	UNP Q9LCB8
B	0	GLY	-	expression tag	UNP Q9LCB8
B	1	SER	-	expression tag	UNP Q9LCB8
B	2	HIS	-	expression tag	UNP Q9LCB8
B	3	HIS	-	expression tag	UNP Q9LCB8
B	4	HIS	-	expression tag	UNP Q9LCB8
B	5	HIS	-	expression tag	UNP Q9LCB8
B	6	HIS	-	expression tag	UNP Q9LCB8
B	7	HIS	-	expression tag	UNP Q9LCB8
B	8	GLY	-	expression tag	UNP Q9LCB8
B	9	MET	-	expression tag	UNP Q9LCB8
B	10	ALA	-	expression tag	UNP Q9LCB8
B	11	SER	-	expression tag	UNP Q9LCB8
B	12	MET	-	expression tag	UNP Q9LCB8
B	13	THR	-	expression tag	UNP Q9LCB8
B	14	GLY	-	expression tag	UNP Q9LCB8
B	15	GLY	-	expression tag	UNP Q9LCB8
B	16	GLN	-	expression tag	UNP Q9LCB8
B	17	GLN	-	expression tag	UNP Q9LCB8
B	18	MET	-	expression tag	UNP Q9LCB8
B	19	GLY	-	expression tag	UNP Q9LCB8
B	20	ARG	-	expression tag	UNP Q9LCB8
B	21	ASP	-	expression tag	UNP Q9LCB8
B	22	LEU	-	expression tag	UNP Q9LCB8
B	23	TYR	-	expression tag	UNP Q9LCB8
B	24	ASP	-	expression tag	UNP Q9LCB8
B	25	ASP	-	expression tag	UNP Q9LCB8
B	26	ASP	-	expression tag	UNP Q9LCB8
B	27	ASP	-	expression tag	UNP Q9LCB8
B	28	LYS	-	expression tag	UNP Q9LCB8

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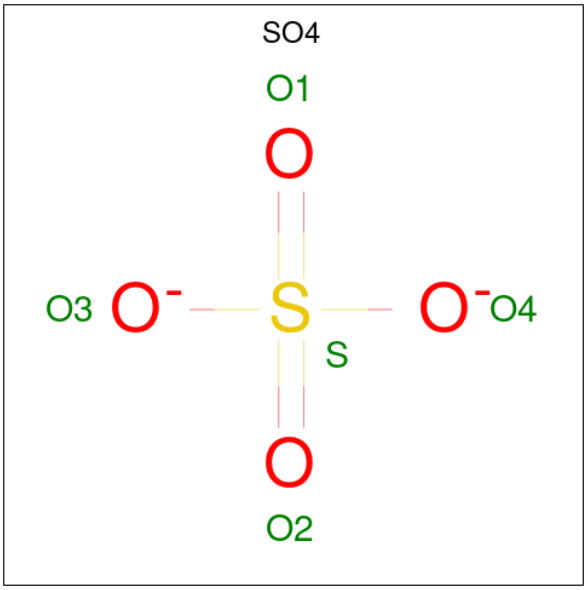
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	ASP	-	expression tag	UNP Q9LCB8
B	30	ARG	-	expression tag	UNP Q9LCB8
B	31	TRP	-	expression tag	UNP Q9LCB8
B	32	GLY	-	expression tag	UNP Q9LCB8
B	33	SER	-	expression tag	UNP Q9LCB8

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

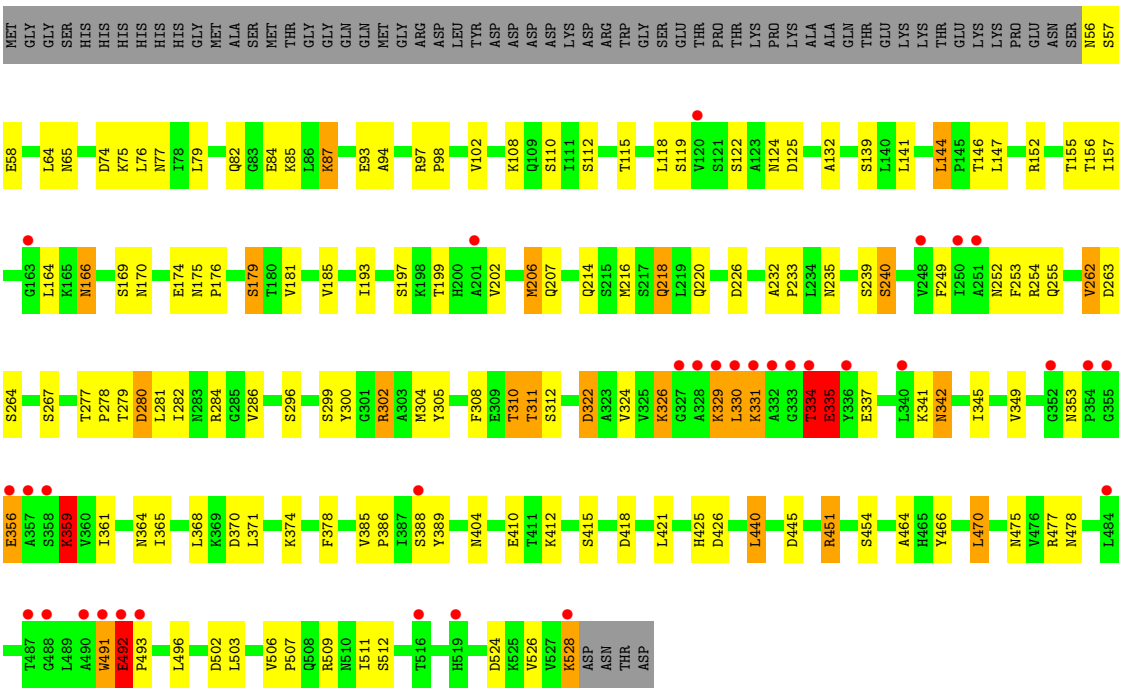
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	205	205	205	0	0
			Total	O		
3	B	246	246	246	0	0

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.

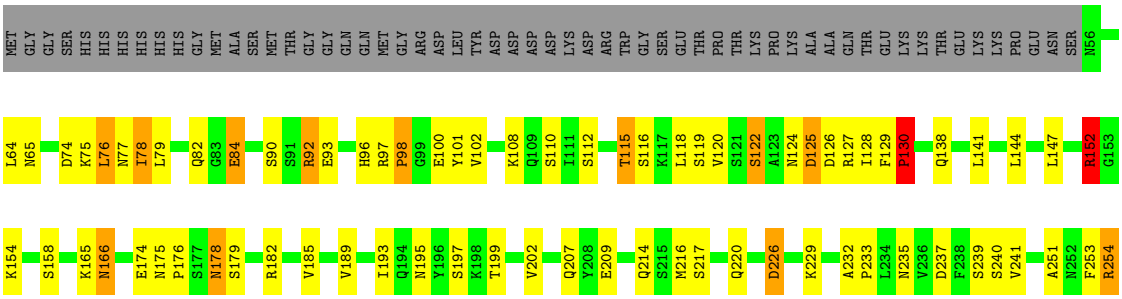
- Molecule 1: intermedilysin

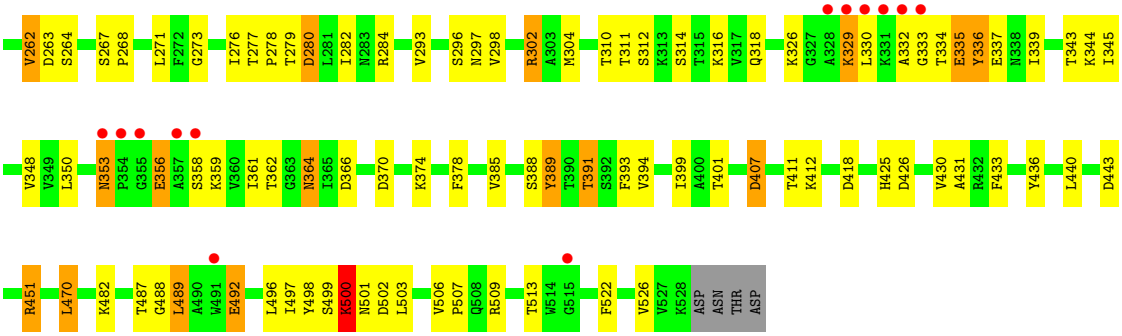
Chain A:



- Molecule 1: intermedilysin

Chain B:




V262 D263 S264 S267 P268 L271 F272 G273 I276 T277 P278 T279 D280 L281 I282 N283 R284 V293 S296 N297 V298 R302 A303 M304 T310 T311 S312 K313 S314 T315 K316 V317 Q318 K326 G327 A328 K329 L330 K331 A332 G333 T334 E335 Y336 E337 N338 I339 T343 K344 I345
V348 V349 L350 N353 P354 G355 E356 A357 S358 K359 V360 I361 T362 G363 N364 I365 D366 D370 K374 F378 V385 S388 Y389 T390 T391 S392 F393 V394 I399 A400 T401 D407 T411 K412 D418 H425 D426 V430 A431 R432 F433 Y436 L440 D443
R451 L470 K482 T487 G488 L489 A490 W491 E492 L496 I497 Y498 S499 K500 N501 D502 L503 V506 P507 Q508 R509 T513 W514 G515 F522 V526 V527 K528 ASP ASN THR ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	88.45Å 173.64Å 105.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.97 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.60) 99.8 (29.97-2.59)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.229 , 0.295 0.238 , 0.307	Depositor DCC
R_{free} test set	2603 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	68.4	Xtriage
Anisotropy	0.837	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7827	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.71	0/3755	0.83	10/5097 (0.2%)
1	B	0.93	6/3755 (0.2%)	0.92	11/5097 (0.2%)
All	All	0.83	6/7510 (0.1%)	0.88	21/10194 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	PRO	CG-CD	8.21	1.77	1.50
1	B	391	THR	CB-CG2	7.71	1.77	1.52
1	B	178	ASN	CG-ND2	7.02	1.50	1.32
1	B	389	TYR	CE1-CZ	-6.95	1.29	1.38
1	B	298	VAL	CB-CG1	5.93	1.65	1.52
1	B	127	ARG	CB-CG	5.18	1.66	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	226	ASP	CB-CG-OD2	7.17	124.76	118.30
1	A	502	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	418	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	370	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	418	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	445	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	280	ASP	CB-CG-OD2	5.76	123.49	118.30
1	B	443	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	370	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	254	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	A	263	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	524	ASP	CB-CG-OD2	5.47	123.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	130	PRO	N-CD-CG	-5.40	95.10	103.20
1	B	407	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	152	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	426	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	366	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	237	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	280	ASP	CB-CG-OD2	5.08	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3678	0	3670	94	0
1	B	3678	0	3670	100	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	205	0	0	24	1
3	B	246	0	0	31	0
All	All	7827	0	7340	193	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 13.

All (193) 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:B:391:THR:CB	1:B:391:THR:CG2	1.77	1.55
1:B:130:PRO:CD	1:B:130:PRO:CG	1.77	1.42
1:B:152:ARG:HD3	3:B:1168:HOH:O	1.51	1.09
1:B:82:GLN:HG2	3:B:1221:HOH:O	1.61	0.97
1:B:138:GLN:HG2	3:B:1250:HOH:O	1.70	0.92
1:A:214:GLN:H	1:A:218:GLN:HE21	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASP:O	1:A:326:LYS:HG2	1.77	0.84
1:B:178:ASN:O	1:B:182:ARG:HG3	1.78	0.83
1:A:119:SER:HB3	1:A:254:ARG:HH21	1.44	0.83
1:A:170:ASN:HB3	3:A:1140:HOH:O	1.81	0.81
1:B:487:THR:O	1:B:489:LEU:N	2.15	0.78
1:B:78:ILE:HA	3:B:1055:HOH:O	1.83	0.77
3:A:1166:HOH:O	1:B:451:ARG:HD3	1.85	0.76
1:A:252:ASN:ND2	1:A:305:TYR:CE2	2.55	0.73
1:B:391:THR:CG2	1:B:391:THR:CA	2.66	0.73
1:A:146:THR:HB	3:A:1186:HOH:O	1.88	0.72
1:B:277:THR:HG22	1:B:279:THR:H	1.57	0.70
1:B:506:VAL:HG11	1:B:526:VAL:HG13	1.75	0.68
1:A:252:ASN:ND2	1:A:305:TYR:CZ	2.62	0.68
1:A:214:GLN:N	1:A:218:GLN:HE21	1.91	0.67
1:A:65:ASN:OD1	1:A:267:SER:HB2	1.95	0.67
1:A:404:ASN:HB3	3:A:1061:HOH:O	1.94	0.66
1:B:65:ASN:OD1	1:B:267:SER:HB2	1.95	0.66
1:A:280:ASP:O	1:A:284:ARG:HD3	1.95	0.65
1:B:232:ALA:HB3	1:B:233:PRO:HD3	1.79	0.65
1:B:482:LYS:HE2	3:B:1192:HOH:O	1.97	0.65
1:A:119:SER:HB3	1:A:254:ARG:NH2	2.11	0.64
1:B:263:ASP:HA	3:B:1125:HOH:O	1.97	0.64
1:A:277:THR:HG22	1:A:279:THR:H	1.61	0.64
1:B:129:PHE:CD1	1:B:178:ASN:HA	2.33	0.63
1:A:506:VAL:HG11	1:A:526:VAL:HG13	1.80	0.62
1:A:342:ASN:HD22	1:A:342:ASN:C	2.03	0.62
1:A:264:SER:HB3	3:A:1090:HOH:O	2.00	0.61
1:A:302:ARG:NH1	3:A:1037:HOH:O	2.30	0.61
1:B:364:ASN:H	1:B:364:ASN:HD22	1.48	0.61
1:A:216:MET:O	1:A:220:GLN:HG3	2.01	0.59
1:A:278:PRO:O	1:A:282:ILE:HG12	2.03	0.58
1:B:84:GLU:HG3	3:B:1124:HOH:O	2.03	0.58
1:A:308:PHE:CD2	1:A:345:ILE:HD11	2.38	0.58
1:A:193:ILE:HA	1:A:197:SER:HB3	1.86	0.58
1:B:278:PRO:O	1:B:282:ILE:HG12	2.04	0.57
1:B:129:PHE:CD1	3:B:1074:HOH:O	2.58	0.57
1:A:181:VAL:O	1:A:185:VAL:HG23	2.06	0.56
1:B:280:ASP:O	1:B:284:ARG:HD3	2.06	0.56
1:B:124:ASN:O	1:B:125:ASP:C	2.42	0.56
1:B:122:SER:N	3:B:1153:HOH:O	2.39	0.56
1:B:193:ILE:HA	1:B:197:SER:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LEU:HD12	1:B:394:VAL:HG13	1.89	0.55
1:B:125:ASP:O	1:B:182:ARG:NH2	2.39	0.55
1:B:358:SER:HB3	3:B:1161:HOH:O	2.07	0.55
1:B:77:ASN:HB3	3:B:1011:HOH:O	2.05	0.55
1:A:361:ILE:HG21	1:A:371:LEU:HD11	1.89	0.54
1:A:82:GLN:HB2	3:A:1059:HOH:O	2.08	0.53
1:B:96:HIS:HD1	1:B:101:TYR:HD1	1.57	0.53
1:A:331:LYS:HD2	1:A:335:GLU:OE2	2.07	0.53
1:B:178:ASN:O	1:B:182:ARG:CG	2.51	0.53
1:A:56:ASN:N	3:A:1033:HOH:O	2.41	0.52
1:B:74:ASP:O	1:B:78:ILE:HG22	2.10	0.52
1:B:329:LYS:HB2	3:B:1173:HOH:O	2.09	0.52
1:B:207:GLN:HE22	1:B:254:ARG:HH11	1.57	0.52
1:B:501:ASN:N	1:B:501:ASN:HD22	2.07	0.52
1:B:316:LYS:HD2	1:B:335:GLU:OE2	2.10	0.52
1:B:119:SER:HB3	1:B:254:ARG:HH21	1.74	0.51
1:B:195:ASN:ND2	3:B:1156:HOH:O	2.29	0.51
1:B:496:LEU:HD23	1:B:497:ILE:N	2.25	0.51
1:B:124:ASN:O	1:B:126:ASP:N	2.44	0.51
1:A:304:MET:HE2	1:A:349:VAL:HG12	1.92	0.51
1:A:57:SER:HA	3:A:1138:HOH:O	2.10	0.50
1:B:425:HIS:CD2	1:B:431:ALA:HB3	2.46	0.50
1:B:97:ARG:O	1:B:98:PRO:C	2.50	0.50
1:B:110:SER:HB3	1:B:407:ASP:OD1	2.11	0.50
1:A:207:GLN:HB3	1:A:254:ARG:HB2	1.92	0.50
1:A:329:LYS:HG3	1:A:330:LEU:H	1.76	0.50
1:B:498:TYR:CD1	1:B:522:PHE:CE1	3.00	0.50
1:B:293:VAL:HG12	1:B:393:PHE:HA	1.94	0.49
1:B:129:PHE:CE1	3:B:1074:HOH:O	2.55	0.49
1:B:470:LEU:HD23	1:B:470:LEU:N	2.28	0.49
1:A:334:THR:HG22	1:A:334:THR:O	2.13	0.49
1:A:253:PHE:HB2	1:A:304:MET:HG2	1.94	0.49
1:B:262:VAL:HG13	1:B:296:SER:HA	1.95	0.48
1:B:273:GLY:O	1:B:276:ILE:HG12	2.13	0.48
1:B:330:LEU:HD23	3:B:1202:HOH:O	2.14	0.48
1:A:74:ASP:CG	1:A:77:ASN:HB2	2.34	0.48
1:B:302:ARG:HD3	3:B:1017:HOH:O	2.14	0.48
1:A:262:VAL:HG13	1:A:296:SER:HA	1.96	0.48
1:B:129:PHE:CD2	1:B:178:ASN:HB2	2.49	0.48
1:B:451:ARG:HG2	3:B:1031:HOH:O	2.12	0.48
1:A:359:LYS:HA	3:A:1089:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASN:HB2	3:A:1121:HOH:O	2.14	0.47
1:B:79:LEU:C	1:B:141:LEU:HD21	2.35	0.47
1:A:85:LYS:HE2	3:B:1247:HOH:O	2.13	0.47
1:A:324:VAL:HG21	1:A:365:ILE:HD11	1.97	0.47
1:A:334:THR:C	1:A:335:GLU:HG3	2.33	0.47
1:A:349:VAL:O	1:A:356:GLU:HG2	2.15	0.47
1:B:175:ASN:O	1:B:176:PRO:C	2.52	0.47
1:B:499:SER:O	1:B:500:LYS:HB2	2.15	0.47
1:A:503:LEU:HD22	1:A:509:ARG:CZ	2.45	0.47
1:A:249:PHE:HB2	1:A:308:PHE:HB2	1.96	0.47
1:A:87:LYS:HE3	1:B:92:ARG:NH1	2.30	0.46
1:A:507:PRO:HG2	1:A:528:LYS:HG2	1.95	0.46
1:B:297:ASN:HB3	3:B:1218:HOH:O	2.14	0.46
1:A:451:ARG:HD3	3:B:1124:HOH:O	2.15	0.46
1:B:175:ASN:HB3	3:B:1205:HOH:O	2.15	0.46
1:A:353:ASN:O	1:A:356:GLU:OE1	2.34	0.46
1:A:359:LYS:HB3	3:A:1074:HOH:O	2.16	0.45
1:B:116:SER:O	1:B:118:LEU:HG	2.16	0.45
1:B:482:LYS:HE3	3:B:1056:HOH:O	2.16	0.45
1:A:281:LEU:HB3	1:A:286:VAL:HB	1.98	0.45
1:A:478:ASN:HA	3:A:1054:HOH:O	2.16	0.45
1:B:356:GLU:O	1:B:359:LYS:O	2.34	0.45
1:A:206:MET:HE1	1:A:255:GLN:HG3	1.98	0.45
1:A:425:HIS:HB3	1:A:466:TYR:HB3	1.99	0.45
1:B:129:PHE:CG	1:B:178:ASN:HA	2.52	0.45
1:B:364:ASN:HD22	1:B:364:ASN:N	2.12	0.45
1:A:79:LEU:C	1:A:141:LEU:HD21	2.37	0.45
1:A:342:ASN:O	1:A:342:ASN:ND2	2.49	0.45
1:B:216:MET:O	1:B:220:GLN:HG3	2.17	0.45
1:A:310:THR:HG22	1:A:342:ASN:HD21	1.82	0.45
1:A:139:SER:HB3	1:A:144:LEU:O	2.17	0.45
1:B:165:LYS:O	1:B:166:ASN:HB2	2.17	0.45
1:A:156:THR:HG23	3:A:1140:HOH:O	2.16	0.44
1:A:326:LYS:O	1:A:326:LYS:HG3	2.16	0.44
1:A:240:SER:HA	3:A:1144:HOH:O	2.18	0.44
1:A:331:LYS:HA	3:A:1157:HOH:O	2.18	0.44
1:A:491:TRP:O	1:A:492:GLU:CB	2.66	0.44
1:B:185:VAL:O	1:B:189:VAL:HG23	2.18	0.44
1:A:58:GLU:HG3	3:A:1194:HOH:O	2.17	0.44
1:A:451:ARG:HG2	3:A:1118:HOH:O	2.17	0.44
1:B:120:VAL:HG23	1:B:388:SER:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:O	1:A:176:PRO:C	2.56	0.44
1:B:489:LEU:HD12	1:B:492:GLU:O	2.17	0.44
1:B:128:ILE:HD12	1:B:389:TYR:CD1	2.53	0.44
1:B:326:LYS:HG2	1:B:326:LYS:O	2.18	0.44
1:A:421:LEU:HD11	1:A:511:ILE:HD12	1.99	0.44
1:A:94:ALA:HA	1:A:102:VAL:O	2.17	0.43
1:B:336:TYR:O	1:B:337:GLU:C	2.57	0.43
1:B:389:TYR:CD2	1:B:389:TYR:N	2.84	0.43
1:A:155:THR:HG22	1:A:157:ILE:HG13	2.00	0.43
1:A:166:ASN:HD22	1:A:166:ASN:N	2.14	0.43
1:A:84:GLU:HG3	3:A:1170:HOH:O	2.17	0.43
1:A:124:ASN:OD1	1:A:124:ASN:C	2.57	0.43
1:B:128:ILE:HD12	1:B:389:TYR:CE1	2.54	0.43
1:B:353:ASN:ND2	1:B:356:GLU:OE1	2.50	0.43
1:A:304:MET:HB3	1:A:349:VAL:HG12	2.01	0.43
1:B:65:ASN:OD1	1:B:268:PRO:HD2	2.17	0.43
1:B:97:ARG:O	1:B:98:PRO:O	2.37	0.43
1:B:78:ILE:CA	3:B:1055:HOH:O	2.55	0.43
1:B:122:SER:HB3	3:B:1180:HOH:O	2.18	0.43
1:B:120:VAL:HG23	1:B:388:SER:CA	2.49	0.42
1:A:179:SER:HB2	3:A:1005:HOH:O	2.17	0.42
1:B:229:LYS:HG3	3:B:1089:HOH:O	2.18	0.42
1:B:318:GLN:HB3	3:B:1181:HOH:O	2.20	0.42
1:A:410:GLU:HG2	3:A:1205:HOH:O	2.19	0.42
1:B:209:GLU:O	1:B:251:ALA:HA	2.18	0.42
1:A:84:GLU:HA	3:A:1065:HOH:O	2.18	0.42
1:A:119:SER:CB	1:A:254:ARG:HH21	2.25	0.42
1:A:302:ARG:NH2	1:A:304:MET:HE1	2.34	0.42
1:A:426:ASP:HA	1:A:464:ALA:O	2.18	0.42
1:A:132:ALA:HB1	1:A:147:LEU:HD21	2.01	0.42
1:A:164:LEU:HD13	1:A:169:SER:HA	2.01	0.42
1:A:342:ASN:C	1:A:342:ASN:ND2	2.72	0.42
1:B:214:GLN:HA	3:B:1019:HOH:O	2.19	0.42
1:B:503:LEU:HD22	1:B:509:ARG:CZ	2.50	0.42
1:A:491:TRP:O	1:A:492:GLU:HB3	2.18	0.42
1:B:253:PHE:HB2	1:B:304:MET:HG2	2.00	0.42
1:A:361:ILE:HD12	3:A:1204:HOH:O	2.19	0.42
1:A:368:LEU:O	1:A:371:LEU:N	2.53	0.42
1:B:202:VAL:HB	1:B:378:PHE:HB3	2.01	0.42
1:B:506:VAL:HG13	1:B:507:PRO:HD2	2.02	0.42
1:B:120:VAL:HG23	1:B:388:SER:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HB2	1:B:389:TYR:CE2	2.55	0.41
1:B:78:ILE:O	1:B:78:ILE:HG12	2.20	0.41
1:B:77:ASN:CB	3:B:1011:HOH:O	2.67	0.41
1:B:115:THR:HG21	3:B:1085:HOH:O	2.19	0.41
1:A:310:THR:HG22	1:A:342:ASN:ND2	2.35	0.41
1:A:337:GLU:O	1:A:341:LYS:HG3	2.21	0.41
1:B:75:LYS:O	1:B:77:ASN:N	2.54	0.41
1:B:507:PRO:HD3	3:B:1012:HOH:O	2.20	0.41
1:A:206:MET:CE	1:A:255:GLN:HG3	2.51	0.41
1:B:74:ASP:O	1:B:75:LYS:C	2.59	0.41
1:A:311:THR:HG22	3:A:1120:HOH:O	2.20	0.41
1:A:232:ALA:HB3	1:A:233:PRO:HD3	2.02	0.41
1:A:118:LEU:HD12	1:A:389:TYR:CE1	2.55	0.41
1:A:202:VAL:HB	1:A:378:PHE:HB3	2.03	0.41
1:B:326:LYS:O	1:B:326:LYS:CG	2.68	0.41
1:B:430:VAL:HG23	3:B:1122:HOH:O	2.20	0.41
1:A:440:LEU:O	1:A:475:ASN:ND2	2.45	0.40
1:A:470:LEU:HD23	1:A:470:LEU:N	2.37	0.40
1:A:299:SER:HB2	1:A:388:SER:OG	2.21	0.40
1:A:300:TYR:CE2	1:A:386:PRO:HG3	2.56	0.40
1:A:214:GLN:HB2	1:A:218:GLN:NE2	2.37	0.40
1:B:241:VAL:O	1:B:411:THR:HG21	2.21	0.40
1:B:433:PHE:CD1	1:B:433:PHE:N	2.87	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:A:1016:HOH:O	3:A:1136:HOH:O[3_546]	2.19	0.01

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	471/535 (88%)	421 (89%)	41 (9%)	9 (2%)	8 15
1	B	471/535 (88%)	414 (88%)	43 (9%)	14 (3%)	4 7
All	All	942/1070 (88%)	835 (89%)	84 (9%)	23 (2%)	6 10

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	98	PRO
1	B	125	ASP
1	B	329	LYS
1	B	333	GLY
1	B	488	GLY
1	A	235	ASN
1	A	329	LYS
1	A	334	THR
1	B	76	LEU
1	B	78	ILE
1	B	235	ASN
1	B	500	LYS
1	A	75	LYS
1	A	335	GLU
1	A	359	LYS
1	B	130	PRO
1	B	166	ASN
1	B	226	ASP
1	B	332	ALA
1	A	492	GLU
1	A	496	LEU
1	B	336	TYR
1	A	493	PRO

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	405/457 (89%)	358 (88%)	47 (12%)	5 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	405/457 (89%)	346 (85%)	59 (15%)	3 5
All	All	810/914 (89%)	704 (87%)	106 (13%)	4 7

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LEU
1	A	76	LEU
1	A	87	LYS
1	A	93	GLU
1	A	97	ARG
1	A	98	PRO
1	A	108	LYS
1	A	110	SER
1	A	112	SER
1	A	115	THR
1	A	122	SER
1	A	144	LEU
1	A	152	ARG
1	A	166	ASN
1	A	174	GLU
1	A	179	SER
1	A	199	THR
1	A	206	MET
1	A	218	GLN
1	A	239	SER
1	A	240	SER
1	A	262	VAL
1	A	302	ARG
1	A	310	THR
1	A	311	THR
1	A	312	SER
1	A	326	LYS
1	A	330	LEU
1	A	331	LYS
1	A	334	THR
1	A	335	GLU
1	A	342	ASN
1	A	356	GLU
1	A	359	LYS
1	A	374	LYS
1	A	385	VAL

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Mol	Chain	Res	Type
1	A	412	LYS
1	A	415	SER
1	A	440	LEU
1	A	451	ARG
1	A	454	SER
1	A	470	LEU
1	A	477	ARG
1	A	491	TRP
1	A	492	GLU
1	A	512	SER
1	A	528	LYS
1	B	64	LEU
1	B	76	LEU
1	B	84	GLU
1	B	90	SER
1	B	92	ARG
1	B	93	GLU
1	B	100	GLU
1	B	102	VAL
1	B	108	LYS
1	B	112	SER
1	B	115	THR
1	B	122	SER
1	B	130	PRO
1	B	144	LEU
1	B	147	LEU
1	B	152	ARG
1	B	154	LYS
1	B	158	SER
1	B	174	GLU
1	B	179	SER
1	B	199	THR
1	B	217	SER
1	B	226	ASP
1	B	239	SER
1	B	240	SER
1	B	262	VAL
1	B	264	SER
1	B	302	ARG
1	B	310	THR
1	B	311	THR
1	B	312	SER

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Mol	Chain	Res	Type
1	B	314	SER
1	B	334	THR
1	B	335	GLU
1	B	339	ILE
1	B	343	THR
1	B	344	LYS
1	B	345	ILE
1	B	348	VAL
1	B	350	LEU
1	B	353	ASN
1	B	356	GLU
1	B	361	ILE
1	B	362	THR
1	B	364	ASN
1	B	374	LYS
1	B	385	VAL
1	B	399	ILE
1	B	401	THR
1	B	412	LYS
1	B	436	TYR
1	B	440	LEU
1	B	451	ARG
1	B	470	LEU
1	B	489	LEU
1	B	492	GLU
1	B	500	LYS
1	B	502	ASP
1	B	513	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	207	GLN
1	A	218	GLN
1	A	220	GLN
1	A	318	GLN
1	A	342	ASN
1	A	501	ASN
1	B	82	GLN
1	B	89	HIS
1	B	166	ASN

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Mol	Chain	Res	Type
1	B	170	ASN
1	B	200	HIS
1	B	207	GLN
1	B	220	GLN
1	B	318	GLN
1	B	364	ASN
1	B	501	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 monosaccharides 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	SO4	B	1003	-	4,4,4	0.20	0	6,6,6	0.64	0
2	SO4	A	1001	-	4,4,4	0.16	0	6,6,6	0.30	0
2	SO4	A	1002	-	4,4,4	0.17	0	6,6,6	0.46	0
2	SO4	B	1004	-	4,4,4	0.18	0	6,6,6	0.54	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	473/535 (88%)	0.18	33 (6%)	16	12	25, 39, 49, 61	0
1	B	473/535 (88%)	-0.02	13 (2%)	54	48	15, 37, 48, 58	0
All	All	946/1070 (88%)	0.08	46 (4%)	29	23	15, 38, 48, 61	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	PRO	6.5
1	A	488	GLY	6.3
1	B	330	LEU	5.2
1	A	332	ALA	4.9
1	B	355	GLY	4.3
1	A	355	GLY	4.2
1	A	490	ALA	4.1
1	A	331	LYS	4.0
1	B	331	LYS	3.9
1	A	484	LEU	3.8
1	B	333	GLY	3.8
1	A	250	ILE	3.6
1	A	201	ALA	3.5
1	A	334	THR	3.5
1	B	329	LYS	3.5
1	A	333	GLY	3.5
1	A	358	SER	3.4
1	A	356	GLU	3.3
1	A	357	ALA	3.3
1	A	330	LEU	3.2
1	B	332	ALA	3.1
1	B	358	SER	3.1
1	A	491	TRP	3.0
1	A	519	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	353	ASN	2.9
1	A	251	ALA	2.8
1	A	336	TYR	2.8
1	A	352	GLY	2.7
1	B	354	PRO	2.6
1	B	328	ALA	2.6
1	B	491	TRP	2.5
1	A	492	GLU	2.4
1	B	515	GLY	2.4
1	A	327	GLY	2.3
1	A	388	SER	2.3
1	A	516	THR	2.3
1	A	329	LYS	2.2
1	A	487	THR	2.2
1	A	340	LEU	2.1
1	A	120	VAL	2.1
1	A	163	GLY	2.1
1	A	528	LYS	2.1
1	A	328	ALA	2.1
1	B	357	ALA	2.1
1	A	248	VAL	2.1
1	A	493	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	1003	5/5	0.95	0.27	44,44,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	1004	5/5	0.95	0.38	42,43,46,46	0
2	SO4	A	1001	5/5	0.96	0.45	45,46,47,48	0
2	SO4	A	1002	5/5	0.97	0.29	47,50,51,52	0

6.5 Other polymers (i)

There are no such residues in this entry.