Full wwPDB X-ray Structure Validation Report (i)

Sep 27, 2022 – 10:50 am BST

PDB ID	:	7ZML
Title	:	Crystal structure of human RECQL5 helicase APO form in complex with engineered nanobody (Gluebody) G1-001
Authors	:	Ye, M.; Makola, M.; Newman, J.A.; Fairhead, M.; MacLean, E.; Krojer, T.; Aitkenhead, H.; Bountra, C.; Gileadi, O.; von Delft, F.
Deposited on	:	2022-04-19
Resolution	:	2.79 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:

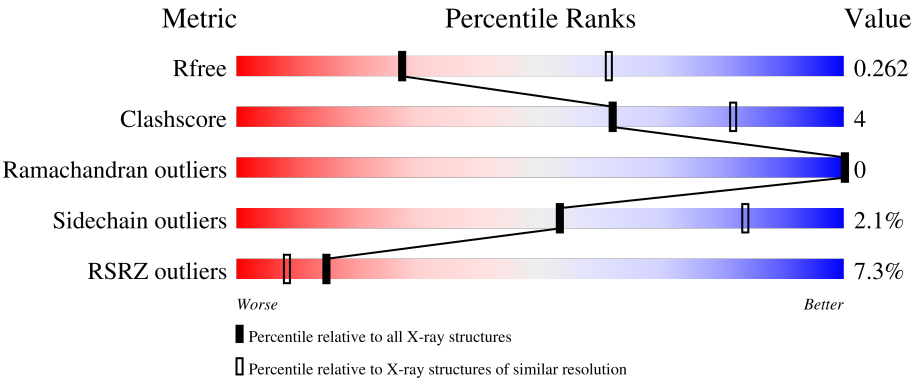
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	445	3% 85% 14%
1	B	445	6% 87% 11%
1	C	445	8% 86% 13%
1	D	445	17% 85% 14%
2	E	132	3% 88% 7%

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Mol	Chain	Length	Quality of chain
2	F	132	8% 88% 11%
2	G	132	4% 86% 14%
2	K	132	88% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	502	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17730 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 ATP-dependent DNA helicase Q5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	4	0
			3452	2180	622	627	23			
1	B	441	Total	C	N	O	S	0	4	0
			3409	2155	605	626	23			
1	C	441	Total	C	N	O	S	0	5	0
			3432	2169	612	628	23			
1	D	440	Total	C	N	O	S	0	5	0
			3452	2180	623	626	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	SER	-	expression tag	UNP O94762
A	10	MET	-	expression tag	UNP O94762
B	9	SER	-	expression tag	UNP O94762
B	10	MET	-	expression tag	UNP O94762
C	9	SER	-	expression tag	UNP O94762
C	10	MET	-	expression tag	UNP O94762
D	9	SER	-	expression tag	UNP O94762
D	10	MET	-	expression tag	UNP O94762

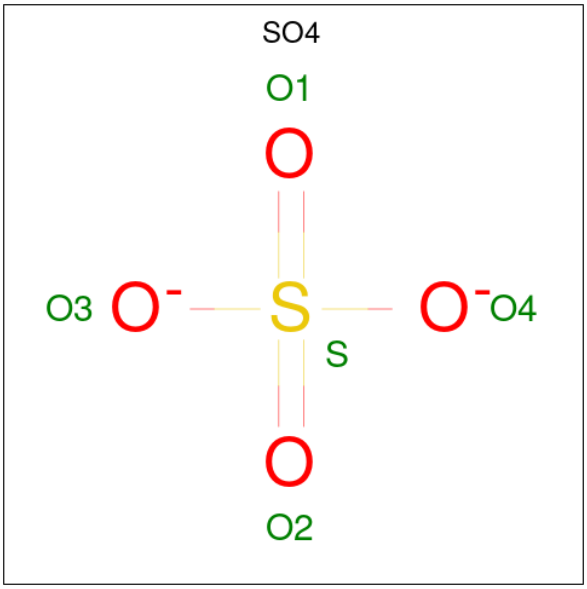
- Molecule 2 is a protein called Gluebody G1-001.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	131	Total	C	N	O	S	0	0	0
			996	623	169	200	4			
2	E	128	Total	C	N	O	S	0	0	0
			965	599	166	196	4			
2	F	130	Total	C	N	O	S	0	0	0
			985	614	168	199	4			
2	G	131	Total	C	N	O	S	0	0	0
			996	623	169	200	4			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

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

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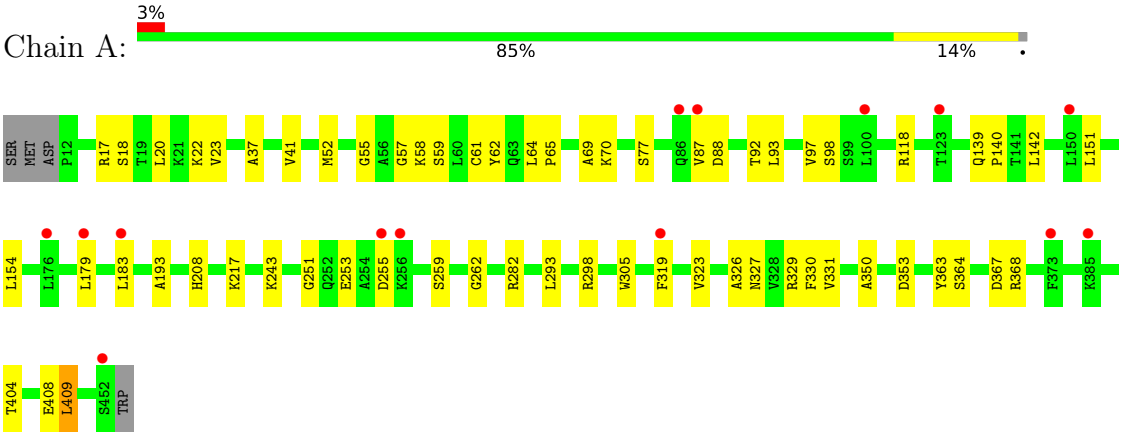
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	6	Total O 6 6	0	0
5	C	2	Total O 2 2	0	0
5	D	2	Total O 2 2	0	0
5	K	1	Total O 1 1	0	0
5	E	3	Total O 3 3	0	0
5	G	2	Total O 2 2	0	0

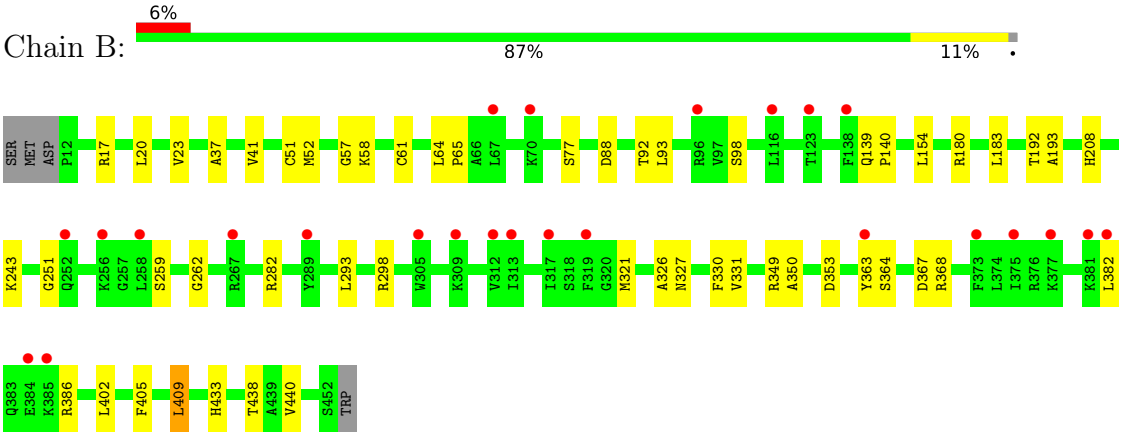
3 Residue-property plots (i)

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.

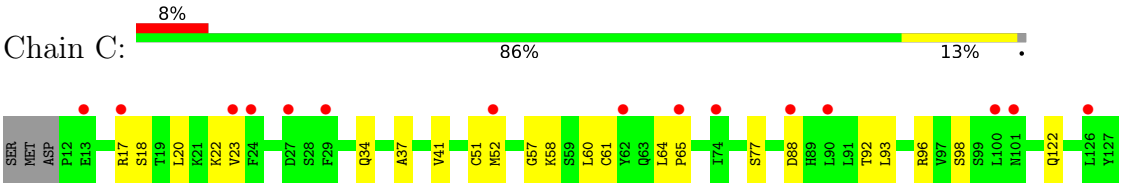
• Molecule 1: ATP-dependent DNA helicase Q5

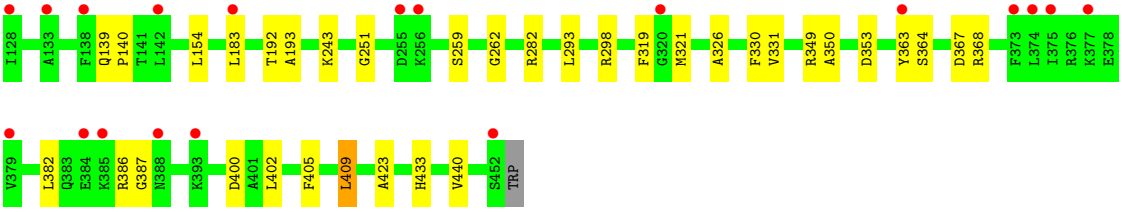


• Molecule 1: ATP-dependent DNA helicase Q5

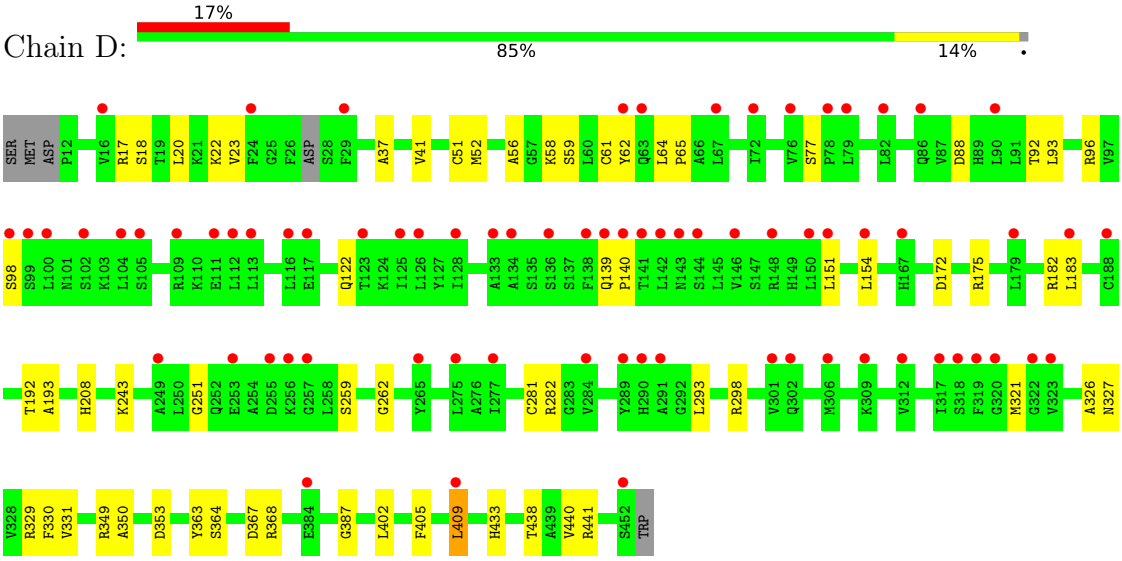


• Molecule 1: ATP-dependent DNA helicase Q5

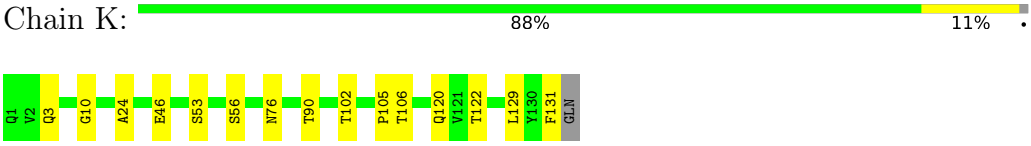




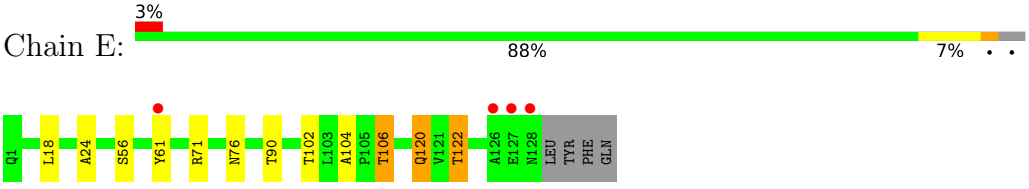
• Molecule 1: ATP-dependent DNA helicase Q5



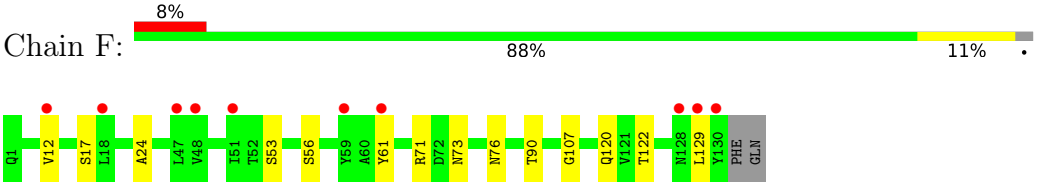
• Molecule 2: Gluebody G1-001



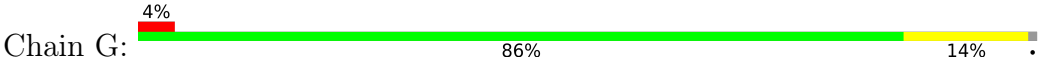
• Molecule 2: Gluebody G1-001



• Molecule 2: Gluebody G1-001



• Molecule 2: Gluebody G1-001




Q1
E6
A24
W36
S53
S56
K64
I69
N76
T77
V78
Y79
T90
T106
G116
Q120
V121
T122
V123
S124
E127
N128
L129
Y130
F131
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.74Å 185.53Å 101.01Å 90.00° 107.47° 90.00°	Depositor
Resolution (Å)	96.35 – 2.79 96.35 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.6 (96.35-2.79) 99.6 (96.35-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.224 , 0.261 0.227 , 0.262	Depositor DCC
R_{free} test set	3147 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	89.5	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17730	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN

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	0.67	0/3528	0.84	0/4766
1	B	0.67	0/3504	0.81	0/4738
1	C	0.67	0/3525	0.81	0/4764
1	D	0.66	0/3526	0.80	0/4761
2	E	0.67	0/983	0.87	1/1332 (0.1%)
2	F	0.67	0/1004	0.85	0/1361
2	G	0.67	0/1016	0.86	0/1377
2	K	0.68	0/1016	0.87	0/1377
All	All	0.67	0/18102	0.83	1/24476 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	71	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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	3452	0	3484	37	0
1	B	3409	0	3399	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3432	0	3439	31	0
1	D	3452	0	3481	36	0
2	E	965	0	918	5	0
2	F	985	0	938	6	0
2	G	996	0	947	13	0
2	K	996	0	947	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	2	0
4	B	5	0	0	1	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
5	A	3	0	0	1	0
5	B	6	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	G	2	0	0	0	0
5	K	1	0	0	0	0
All	All	17730	0	17553	156	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 4.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:LYS:HD3	1:D:282:ARG:HB3	1.69	0.74
1:A:142:LEU:CD2	1:A:179:LEU:HD11	2.18	0.73
1:B:208:HIS:ND1	1:D:387:GLY:HA3	2.06	0.70
1:D:52:MET:O	1:D:193:ALA:HA	1.92	0.69
2:E:90:THR:HG23	2:E:122:THR:HA	1.76	0.68
1:A:57:GLY:N	4:A:502:SO4:O4	2.26	0.68
1:A:243:LYS:HD3	1:A:282:ARG:HB3	1.74	0.68
1:A:142:LEU:HD21	1:A:179:LEU:HD11	1.76	0.66
1:B:243:LYS:HD3	1:B:282:ARG:HB3	1.78	0.66
1:A:88:ASP:O	1:A:92:THR:HG23	1.98	0.64
2:F:90:THR:HG23	2:F:122:THR:HA	1.79	0.64
1:C:88:ASP:O	1:C:92:THR:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:ASP:O	1:D:92:THR:HG23	2.00	0.61
1:B:88:ASP:O	1:B:92:THR:HG23	2.00	0.61
2:G:36:TRP:HD1	2:G:69:ILE:HD13	1.65	0.61
1:B:409:LEU:HD13	1:B:409:LEU:H	1.67	0.60
2:G:90:THR:HG23	2:G:122:THR:HA	1.82	0.59
1:D:59:SER:HA	1:D:62:TYR:CE2	2.37	0.59
1:D:64:LEU:HB3	1:D:65:PRO:HD3	1.85	0.59
2:G:69:ILE:HD11	2:G:78:VAL:CG2	2.33	0.59
2:K:90:THR:HG23	2:K:122:THR:HA	1.83	0.58
1:C:64:LEU:HB3	1:C:65:PRO:HD3	1.84	0.58
1:B:64:LEU:HB3	1:B:65:PRO:HD3	1.84	0.58
1:B:262:GLY:HA3	1:B:330:PHE:CE2	2.40	0.57
1:A:52:MET:O	1:A:193:ALA:HA	2.04	0.57
1:D:438:THR:HG22	1:D:441[A]:ARG:NH2	2.20	0.57
1:B:154:LEU:HD22	1:B:183:LEU:HD12	1.86	0.56
1:C:409:LEU:H	1:C:409:LEU:HD13	1.70	0.56
1:C:262:GLY:HA3	1:C:330:PHE:CE2	2.41	0.56
1:A:409:LEU:H	1:A:409:LEU:HD13	1.71	0.56
1:D:409:LEU:H	1:D:409:LEU:HD13	1.71	0.56
2:F:71:ARG:HD2	2:F:73:ASN:OD1	2.05	0.56
1:A:262:GLY:HA3	1:A:330:PHE:CE2	2.41	0.55
1:C:57:GLY:N	4:C:502:SO4:O1	2.37	0.55
1:A:64:LEU:HB3	1:A:65:PRO:HD3	1.88	0.55
1:D:251:GLY:H	1:D:259:SER:H	1.55	0.55
1:D:262:GLY:HA3	1:D:330:PHE:CE2	2.41	0.55
1:A:251:GLY:H	1:A:259:SER:H	1.54	0.55
1:D:329:ARG:NH2	1:D:353:ASP:OD2	2.38	0.54
1:A:55:GLY:O	4:A:502:SO4:O4	2.25	0.54
1:B:52:MET:O	1:B:193:ALA:HA	2.06	0.54
1:B:139:GLN:N	1:B:140:PRO:HD2	2.23	0.54
1:C:139:GLN:N	1:C:140:PRO:HD2	2.24	0.53
1:A:139:GLN:N	1:A:140:PRO:HD2	2.24	0.53
1:A:154:LEU:HD22	1:A:183:LEU:HD12	1.90	0.53
1:D:139:GLN:N	1:D:140:PRO:HD2	2.23	0.53
1:C:23:VAL:O	1:C:93:LEU:HD22	2.09	0.53
1:D:23:VAL:O	1:D:93:LEU:HD22	2.08	0.53
1:A:58:LYS:O	1:A:61:CYS:HB2	2.10	0.52
1:D:154:LEU:HD22	1:D:183:LEU:HD12	1.92	0.52
1:A:329:ARG:NH2	1:A:353:ASP:OD2	2.39	0.52
1:C:52:MET:O	1:C:193:ALA:HA	2.09	0.52
1:D:331:VAL:HG23	1:D:350:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:GLY:H	1:B:259:SER:H	1.58	0.52
1:A:217:LYS:O	2:F:107:GLY:HA3	2.10	0.51
2:K:10:GLY:HA2	2:G:131:PHE:CZ	2.46	0.50
1:C:58:LYS:O	1:C:61:CYS:HB2	2.13	0.49
1:C:331:VAL:HG23	1:C:350:ALA:HB2	1.94	0.49
1:A:23:VAL:O	1:A:93:LEU:HD22	2.12	0.49
1:C:154:LEU:HD22	1:C:183:LEU:HD12	1.94	0.49
1:C:251:GLY:H	1:C:259:SER:H	1.61	0.49
1:D:326:ALA:HB1	1:D:353:ASP:HB3	1.95	0.49
1:B:331:VAL:HG23	1:B:350:ALA:HB2	1.94	0.48
1:A:208:HIS:ND1	1:C:387:GLY:HA3	2.27	0.48
1:B:58:LYS:O	1:B:61:CYS:HB2	2.12	0.48
1:B:382:LEU:HD13	1:B:386:ARG:NH1	2.28	0.48
1:C:243:LYS:HD3	1:C:282:ARG:HB3	1.95	0.48
1:B:57:GLY:N	4:B:502:SO4:O1	2.39	0.48
1:D:58:LYS:O	1:D:61:CYS:HB2	2.12	0.48
1:A:331:VAL:HG23	1:A:350:ALA:HB2	1.95	0.48
2:G:24:ALA:HB3	2:G:76:ASN:HB3	1.96	0.48
2:E:120:GLN:OE1	2:E:122:THR:HG23	2.13	0.48
1:B:326:ALA:HB1	1:B:353:ASP:HB3	1.96	0.47
1:C:364:SER:O	1:C:367:ASP:HB2	2.14	0.47
2:K:120:GLN:OE1	2:K:122:THR:HG23	2.14	0.47
2:G:124:SER:HB3	2:G:129:LEU:HD22	1.95	0.47
1:C:326:ALA:HB1	1:C:353:ASP:HB3	1.96	0.47
1:D:364:SER:O	1:D:367:ASP:HB2	2.14	0.47
1:A:326:ALA:HB1	1:A:353:ASP:HB3	1.95	0.47
1:B:363:TYR:OH	1:B:368:ARG:HD3	2.14	0.47
2:F:24:ALA:HB3	2:F:76:ASN:HB3	1.96	0.47
1:A:364:SER:O	1:A:367:ASP:HB2	2.15	0.47
1:B:208:HIS:CE1	1:D:387:GLY:HA3	2.49	0.46
1:B:364:SER:O	1:B:367:ASP:HB2	2.15	0.46
1:B:23:VAL:O	1:B:93:LEU:HD22	2.16	0.46
1:A:363:TYR:OH	1:A:368:ARG:HD3	2.16	0.46
1:C:37:ALA:O	1:C:41:VAL:HG23	2.16	0.46
1:C:400:ASP:OD1	2:F:61:TYR:OH	2.26	0.46
1:B:37:ALA:O	1:B:41:VAL:HG23	2.16	0.46
1:C:293:LEU:O	1:C:298:ARG:NH1	2.49	0.46
1:C:363:TYR:OH	1:C:368:ARG:HD3	2.16	0.45
1:B:386:ARG:O	1:D:208:HIS:CE1	2.69	0.45
1:C:423:ALA:HB3	2:K:105:PRO:HA	1.98	0.45
1:A:293:LEU:O	1:A:298:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:ARG:HD2	1:D:122:GLN:HG3	1.99	0.45
1:D:18:SER:O	1:D:22:LYS:N	2.42	0.45
1:D:58:LYS:HE2	1:D:58:LYS:HB3	1.84	0.45
1:D:37:ALA:O	1:D:41:VAL:HG23	2.17	0.45
1:D:433:HIS:HA	1:D:440:VAL:HG21	1.99	0.45
1:D:363:TYR:OH	1:D:368:ARG:HD3	2.17	0.45
1:D:293:LEU:O	1:D:298:ARG:NH1	2.51	0.44
2:K:24:ALA:HB3	2:K:76:ASN:HB3	1.99	0.44
1:A:253:GLU:HB3	1:A:255:ASP:OD2	2.18	0.44
2:E:18:LEU:HA	2:F:17:SER:O	2.17	0.44
1:A:118[B]:ARG:NE	5:A:601:HOH:O	2.50	0.44
1:B:293:LEU:O	1:B:298:ARG:NH1	2.51	0.44
1:A:17:ARG:O	1:A:20:LEU:HB3	2.18	0.44
1:B:409:LEU:H	1:B:409:LEU:CD1	2.30	0.44
1:C:18:SER:O	1:C:22:LYS:N	2.42	0.44
1:C:34:GLN:HE21	1:C:60:LEU:HD23	1.82	0.44
2:G:36:TRP:CD1	2:G:69:ILE:HD13	2.51	0.44
1:D:172:ASP:CG	1:D:175[B]:ARG:HH22	2.22	0.43
1:A:87:VAL:HG23	1:A:97:VAL:HG22	2.00	0.43
1:C:17:ARG:O	1:C:20:LEU:HB3	2.17	0.43
1:B:402:LEU:O	1:B:405:PHE:HB3	2.18	0.43
1:A:151:LEU:HD21	1:A:183:LEU:HD13	2.01	0.43
1:C:433:HIS:HA	1:C:440:VAL:HG21	2.01	0.43
1:D:17:ARG:O	1:D:20:LEU:HB3	2.19	0.43
1:B:17:ARG:O	1:B:20:LEU:HB3	2.19	0.43
2:K:10:GLY:HA2	2:G:131:PHE:CE1	2.52	0.43
1:B:433:HIS:HA	1:B:440:VAL:HG21	2.01	0.43
1:A:305:TRP:CZ3	1:A:319:PHE:HZ	2.37	0.43
2:G:69:ILE:HD11	2:G:78:VAL:HG21	2.01	0.43
1:A:37:ALA:O	1:A:41:VAL:HG23	2.18	0.42
2:G:129:LEU:HD12	2:G:129:LEU:HA	1.90	0.42
2:G:69:ILE:HD12	2:G:79:TYR:O	2.19	0.42
1:A:142:LEU:HD23	1:A:179:LEU:HD11	1.97	0.42
1:D:321:MET:HB3	1:D:349:ARG:NE	2.34	0.42
1:A:327:ASN:HA	1:A:353:ASP:OD2	2.20	0.42
1:B:321:MET:HB3	1:B:349:ARG:NE	2.34	0.42
1:D:56:ALA:HA	1:D:58:LYS:HE3	2.01	0.42
1:D:402:LEU:O	1:D:405:PHE:HB3	2.20	0.42
2:G:6:GLU:OE1	2:G:116:GLY:HA3	2.20	0.42
1:A:329:ARG:HH22	1:A:353:ASP:CG	2.23	0.41
2:K:120:GLN:HB3	2:G:131:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:104:ALA:O	2:E:106:THR:O	2.38	0.41
1:A:59:SER:HA	1:A:62:TYR:CE2	2.56	0.41
1:C:96:ARG:HD2	1:C:122:GLN:HG3	2.02	0.41
2:E:24:ALA:HB3	2:E:76:ASN:HB3	2.02	0.41
1:C:321:MET:HB3	1:C:349:ARG:NE	2.35	0.41
1:C:402:LEU:O	1:C:405:PHE:HB3	2.21	0.41
2:K:129:LEU:HB3	2:K:131:PHE:CZ	2.56	0.41
1:D:64:LEU:C	1:D:64:LEU:HD23	2.41	0.41
1:A:69:ALA:O	1:A:70:LYS:HB2	2.21	0.40
1:B:321:MET:HB3	1:B:349:ARG:HE	1.87	0.40
1:C:321:MET:HB3	1:C:349:ARG:HE	1.86	0.40
1:D:151:LEU:HD21	1:D:183:LEU:HD13	2.03	0.40
1:B:51:CYS:HA	1:B:192:THR:O	2.21	0.40
1:B:327:ASN:HA	1:B:353:ASP:OD2	2.21	0.40
1:D:327:ASN:HA	1:D:353:ASP:OD2	2.21	0.40
1:A:18:SER:O	1:A:22:LYS:N	2.41	0.40
1:A:404:THR:O	1:A:408:GLU:HG2	2.20	0.40
1:C:51:CYS:HA	1:C:192:THR:O	2.21	0.40
1:C:382:LEU:O	1:C:386:ARG:HG2	2.22	0.40
1:D:51:CYS:HA	1:D:192:THR:O	2.21	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	443/445 (100%)	431 (97%)	12 (3%)	0	100	100
1	B	443/445 (100%)	432 (98%)	11 (2%)	0	100	100
1	C	444/445 (100%)	432 (97%)	12 (3%)	0	100	100
1	D	441/445 (99%)	428 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	126/132 (96%)	124 (98%)	2 (2%)	0	100	100
2	F	128/132 (97%)	126 (98%)	2 (2%)	0	100	100
2	G	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
2	K	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
All	All	2283/2308 (99%)	2223 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	369/373 (99%)	365 (99%)	4 (1%)	73	92
1	B	365/373 (98%)	361 (99%)	4 (1%)	73	92
1	C	368/373 (99%)	364 (99%)	4 (1%)	73	92
1	D	368/373 (99%)	363 (99%)	5 (1%)	67	90
2	E	98/103 (95%)	92 (94%)	6 (6%)	18	48
2	F	100/103 (97%)	95 (95%)	5 (5%)	24	56
2	G	101/103 (98%)	96 (95%)	5 (5%)	24	56
2	K	101/103 (98%)	95 (94%)	6 (6%)	19	49
All	All	1870/1904 (98%)	1831 (98%)	39 (2%)	53	84

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	SER
1	A	98	SER
1	A	323	VAL
1	A	409	LEU
1	B	77	SER
1	B	98	SER

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Mol	Chain	Res	Type
1	B	180	ARG
1	B	409	LEU
1	C	77	SER
1	C	98	SER
1	C	319	PHE
1	C	409	LEU
1	D	77	SER
1	D	98	SER
1	D	182	ARG
1	D	281	CYS
1	D	409	LEU
2	K	3	GLN
2	K	46	GLU
2	K	53	SER
2	K	56	SER
2	K	102	THR
2	K	106	THR
2	E	56	SER
2	E	61	TYR
2	E	102	THR
2	E	106	THR
2	E	120	GLN
2	E	122	THR
2	F	12	VAL
2	F	53	SER
2	F	56	SER
2	F	120	GLN
2	F	129	LEU
2	G	53	SER
2	G	56	SER
2	G	64	LYS
2	G	106	THR
2	G	120	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	285	ASN
1	B	139	GLN
1	B	208	HIS
1	B	285	ASN

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Mol	Chain	Res	Type
1	C	101	ASN
1	C	139	GLN
1	C	208	HIS
1	D	101	ASN
1	D	139	GLN
1	D	208	HIS
1	D	285	ASN
2	K	3	GLN
2	F	3	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
4	SO4	D	502	-	4,4,4	0.30	0	6,6,6	0.23	0
4	SO4	A	502	-	4,4,4	0.31	0	6,6,6	0.26	0
4	SO4	B	502	-	4,4,4	0.44	0	6,6,6	0.09	0
4	SO4	C	502	-	4,4,4	0.32	0	6,6,6	0.21	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	SO4	2	0
4	B	502	SO4	1	0
4	C	502	SO4	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, 95^{th} 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	441/445 (99%)	0.11	14 (3%) 47 37	61, 93, 143, 230	0
1	B	441/445 (99%)	0.29	25 (5%) 23 15	65, 109, 177, 212	0
1	C	441/445 (99%)	0.35	34 (7%) 13 7	65, 113, 180, 206	0
1	D	440/445 (98%)	0.87	74 (16%) 1 1	76, 136, 211, 259	0
2	E	128/132 (96%)	0.19	4 (3%) 49 39	57, 83, 133, 210	0
2	F	130/132 (98%)	0.45	10 (7%) 13 7	55, 82, 131, 243	0
2	G	131/132 (99%)	0.06	5 (3%) 40 30	55, 78, 157, 169	0
2	K	131/132 (99%)	-0.05	0 100 100	58, 74, 105, 134	0
All	All	2283/2308 (98%)	0.35	166 (7%) 15 8	55, 103, 183, 259	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	128	ASN	20.7
1	D	100	LEU	9.7
1	C	320	GLY	9.6
2	F	130	TYR	9.5
2	G	131	PHE	8.4
2	G	129	LEU	8.1
1	D	117	GLU	7.6
1	D	99	SER	6.7
2	G	130	TYR	6.5
1	D	79	LEU	6.4
1	D	136	SER	6.3
1	B	256	LYS	6.2
1	D	126	LEU	6.1
1	D	142	LEU	6.0
1	C	100	LEU	5.9
1	D	146	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	255	ASP	5.5
1	D	123	THR	5.5
1	B	377	LYS	5.5
1	D	104	LEU	5.4
1	D	98	SER	5.4
1	B	382	LEU	5.2
1	D	256	LYS	5.0
1	C	74	ILE	5.0
1	D	109	ARG	4.9
1	D	116	LEU	4.8
2	E	127	GLU	4.8
1	D	113	LEU	4.8
1	B	252	GLN	4.7
1	B	381	LYS	4.6
1	A	183	LEU	4.6
1	D	154	LEU	4.5
1	B	116	LEU	4.3
1	C	90	LEU	4.3
1	B	309	LYS	4.2
1	D	112	LEU	4.2
1	C	24	PHE	4.1
2	F	128	ASN	4.1
1	D	72	ILE	4.0
1	C	385	LYS	3.9
1	A	255	ASP	3.8
1	C	373	PHE	3.8
1	D	144	SER	3.7
1	B	258	LEU	3.7
2	E	61	TYR	3.6
1	D	319	PHE	3.6
1	C	101	ASN	3.6
1	D	318	SER	3.5
1	D	16	VAL	3.5
1	D	90	LEU	3.5
1	D	139	GLN	3.5
1	D	179	LEU	3.5
1	C	138	PHE	3.5
1	D	78	PRO	3.5
1	B	317	ILE	3.4
1	D	291	ALA	3.4
1	A	179	LEU	3.4
2	G	127	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	384	GLU	3.3
1	D	290	HIS	3.3
1	C	126	LEU	3.3
1	C	27	ASP	3.2
1	D	148	ARG	3.2
1	B	385	LYS	3.2
1	C	255	ASP	3.2
1	D	105	SER	3.2
1	D	151	LEU	3.2
1	D	257	GLY	3.2
2	F	51	ILE	3.1
1	C	88	ASP	3.1
1	C	142	LEU	3.1
1	D	128	ILE	3.1
1	C	384	GLU	3.1
1	D	111	GLU	3.0
1	B	138	PHE	3.0
1	C	379	VAL	3.0
1	C	452	SER	3.0
1	D	141	THR	3.0
1	D	183	LEU	3.0
2	E	126	ALA	3.0
1	D	82	LEU	3.0
1	D	167[A]	HIS	2.9
1	D	86	GLN	2.9
1	D	275	LEU	2.9
2	F	129	LEU	2.9
1	C	183	LEU	2.9
1	D	67	LEU	2.9
1	D	62	TYR	2.9
2	F	47	LEU	2.8
1	D	317	ILE	2.8
1	D	138	PHE	2.8
1	D	409	LEU	2.8
1	D	284	VAL	2.8
1	D	63	GLN	2.8
1	A	373	PHE	2.8
1	D	289	TYR	2.7
1	A	256	LYS	2.7
1	C	256	LYS	2.7
1	B	363	TYR	2.7
1	C	128	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	76	VAL	2.7
1	D	322	GLY	2.7
1	A	452	SER	2.6
1	B	96	ARG	2.6
1	D	134	ALA	2.6
1	D	140	PRO	2.6
1	B	312	VAL	2.6
2	F	18	LEU	2.6
1	B	375	ILE	2.5
1	C	133	ALA	2.5
1	A	100	LEU	2.5
1	C	375	ILE	2.5
1	C	374	LEU	2.5
1	A	123	THR	2.5
1	D	249	ALA	2.5
1	D	253	GLU	2.5
2	F	12	VAL	2.5
1	C	377	LYS	2.4
1	D	323	VAL	2.4
1	C	363	TYR	2.4
1	C	23	VAL	2.4
1	D	265	TYR	2.3
1	A	385	LYS	2.3
1	D	125	ILE	2.3
1	A	319	PHE	2.3
1	B	373	PHE	2.3
1	D	29	PHE	2.3
1	D	188	CYS	2.3
1	A	86	GLN	2.3
1	D	24	PHE	2.3
1	C	65	PRO	2.2
1	D	102	SER	2.2
1	D	143	ASN	2.2
1	B	289	TYR	2.2
1	C	62	TYR	2.2
1	D	277	ILE	2.2
1	C	52	MET	2.2
2	F	48	VAL	2.2
1	C	17	ARG	2.2
2	F	61	TYR	2.2
1	D	306	MET	2.2
1	C	388	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	301	VAL	2.2
1	C	29	PHE	2.2
1	D	384	GLU	2.1
1	B	313	ILE	2.1
1	B	67	LEU	2.1
1	B	123	THR	2.1
1	D	309	LYS	2.1
1	B	305	TRP	2.1
2	G	128	ASN	2.1
1	D	452	SER	2.1
1	A	87	VAL	2.1
1	B	267	ARG	2.1
1	D	302	GLN	2.1
1	D	320	GLY	2.1
1	B	70	LYS	2.1
1	B	319	PHE	2.1
1	A	150	LEU	2.0
1	D	150	LEU	2.0
2	F	59	TYR	2.0
1	C	13	GLU	2.0
1	A	176	LEU	2.0
1	C	393	LYS	2.0
1	D	133	ALA	2.0
1	D	312	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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
4	SO4	D	502	5/5	0.86	0.12	130,160,175,187	0
4	SO4	C	502	5/5	0.90	0.11	101,123,142,150	0
3	ZN	A	501	1/1	0.96	0.18	101,101,101,101	0
4	SO4	A	502	5/5	0.96	0.14	73,76,115,120	0
3	ZN	D	501	1/1	0.97	0.12	146,146,146,146	0
4	SO4	B	502	5/5	0.98	0.15	93,103,115,124	0
3	ZN	C	501	1/1	0.99	0.17	102,102,102,102	0
3	ZN	B	501	1/1	1.00	0.20	99,99,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.