



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:02 PM UTC

PDB ID : 7P9M / pdb_00007p9m
Title : BrxU, GmrSD-family Type IV restriction enzyme
Authors : Picton, D.M.; Luyten, Y.; Morgan, R.D.; Nelson, A.; Smith, D.L.; Dryden, D.T.F.; Hinton, J.C.D.; Blower, T.R.
Deposited on : 2021-07-27
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

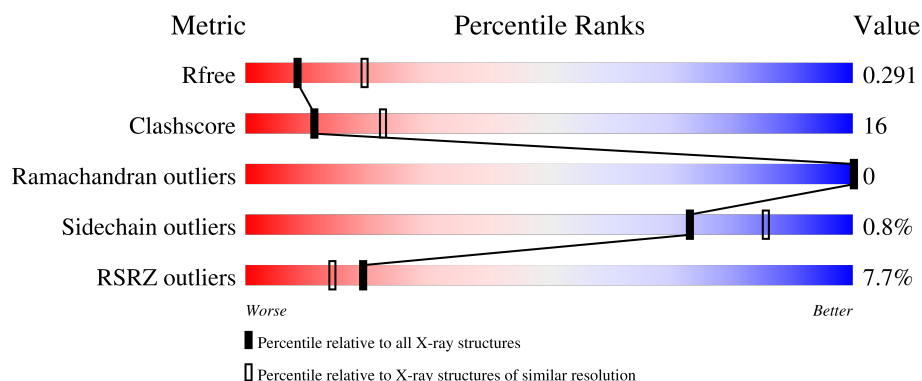
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	587	
1	B	587	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9152 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 DUF262 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	0	0
			4590	2913	804	857	16			
1	B	557	Total	C	N	O	S	0	0	0
			4546	2896	793	842	15			

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



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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

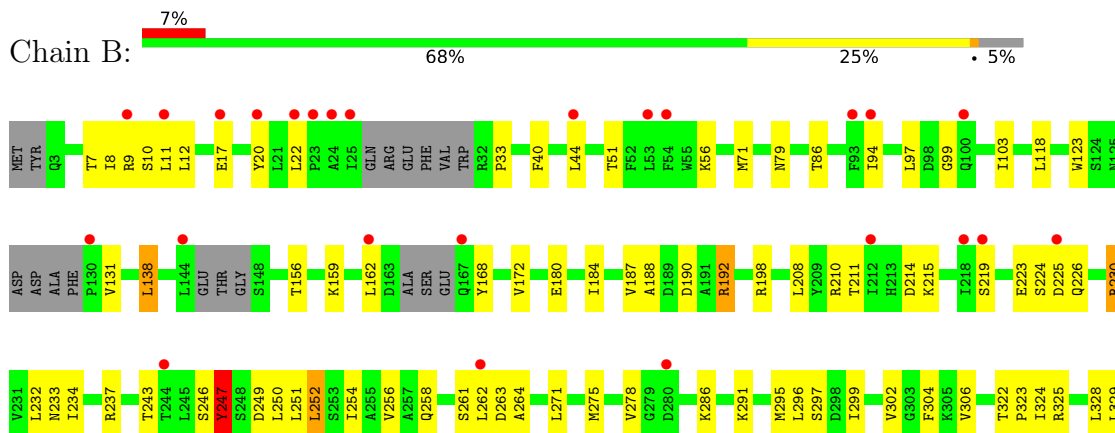
3 Residue-property plots

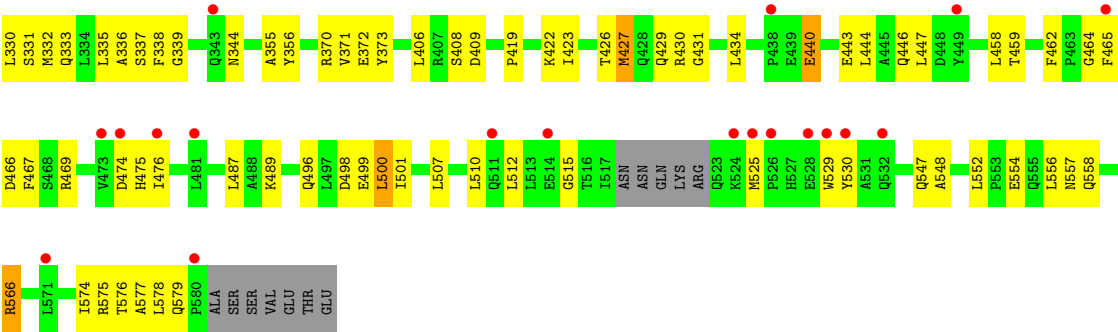
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DUF262 domain-containing protein



• Molecule 1: DUF262 domain-containing protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.88Å 68.37Å 129.59Å 90.00° 94.45° 90.00°	Depositor
Resolution (Å)	98.14 – 2.85 98.14 – 2.85	Depositor Estimate
% Data completeness (in resolution range)	93.4 (98.14-2.85) 93.5 (98.14-2.85)	Depositor Estimate
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.86Å)	Xtriage
Refinement program	REFMAC CCP4 Program Suite v7.1.015, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.266 , 0.278 0.280 , 0.291	Depositor Depositor
R_{free} test set	1914 reflections (4.71%)	wwPDB
Wilson B-factor (Å ²)	98.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.1	Estimate
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	Estimate
Total number of atoms	9152	wwPDB
Average B, all atoms (Å ²)	97.0	wwPDB

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.89	0/4684	1.37	22/6323 (0.3%)
1	B	0.92	1/4643 (0.0%)	1.42	30/6271 (0.5%)
All	All	0.91	1/9327 (0.0%)	1.40	52/12594 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	408	SER	C-O	-5.06	1.18	1.24

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	499	GLU	N-CA-C	-11.79	97.74	114.12
1	B	246	SER	N-CA-C	10.47	123.49	108.00
1	A	105	ALA	N-CA-C	-8.00	103.47	113.55
1	B	247	TYR	N-CA-C	-7.18	103.54	111.36
1	B	500	LEU	N-CA-C	-6.85	105.46	113.88
1	B	138	LEU	N-CA-C	-6.68	103.81	112.23
1	B	337	SER	N-CA-C	-6.40	104.39	111.82
1	A	394	ILE	N-CA-C	-6.27	104.22	110.62
1	B	192	ARG	N-CA-C	-6.23	104.94	112.54
1	B	17	GLU	N-CA-C	-6.20	105.70	113.20
1	B	249	ASP	N-CA-C	-6.19	104.43	112.23
1	A	313	ASN	N-CA-C	-6.13	104.52	111.14
1	A	337	SER	N-CA-C	-6.09	105.81	113.18
1	A	249	ASP	N-CA-C	-6.03	105.91	113.20
1	A	45	GLN	N-CA-C	-6.01	105.70	113.16
1	A	280	ASP	N-CA-C	-6.01	105.80	113.01
1	B	426	THR	N-CA-C	-5.99	104.75	111.28
1	B	262	LEU	N-CA-C	-5.97	106.34	113.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	TYR	N-CA-C	-5.96	105.83	114.12
1	B	33	PRO	CB-CA-C	-5.91	103.67	113.06
1	B	286	LYS	N-CA-C	-5.88	105.21	112.38
1	A	43	LEU	N-CA-C	-5.86	104.89	111.28
1	A	467	PHE	N-CA-C	-5.68	105.45	112.38
1	A	543	HIS	N-CA-C	-5.67	105.10	111.28
1	A	125	ASN	N-CA-C	-5.60	105.26	111.36
1	A	481	LEU	N-CA-C	-5.52	106.54	113.28
1	B	515	GLY	CA-C-O	-5.50	118.17	122.52
1	A	66	GLN	N-CA-C	5.49	118.82	111.24
1	B	338	PHE	N-CA-C	-5.48	106.18	112.92
1	A	149	MET	N-CA-C	-5.48	107.24	114.31
1	A	521	LYS	N-CA-C	-5.42	106.79	113.41
1	B	440	GLU	N-CA-C	-5.39	105.56	111.82
1	B	86	THR	N-CA-C	5.39	116.96	111.14
1	A	304	PHE	N-CA-C	-5.38	107.02	113.21
1	A	435	ARG	N-CA-C	-5.38	100.54	109.46
1	A	106	LEU	N-CA-C	-5.37	105.34	111.14
1	B	246	SER	CB-CA-C	-5.34	108.87	116.34
1	B	344	ASN	CB-CA-C	5.31	117.63	109.03
1	B	232	LEU	N-CA-C	-5.28	105.61	111.36
1	B	372	GLU	N-CA-C	-5.27	106.11	112.54
1	A	372	GLU	N-CA-C	-5.27	106.85	113.28
1	A	571	LEU	N-CA-C	-5.25	105.67	111.71
1	B	547	GLN	N-CA-C	-5.21	106.24	112.59
1	B	230	ARG	CB-CA-C	-5.17	102.77	110.88
1	B	252	LEU	N-CA-C	-5.17	105.54	111.07
1	A	444	LEU	N-CA-C	-5.13	105.87	111.82
1	B	476	ILE	N-CA-C	-5.08	104.95	110.23
1	B	335	LEU	N-CA-C	-5.05	105.85	111.36
1	B	489	LYS	N-CA-C	-5.05	105.78	111.28
1	B	330	LEU	N-CA-C	-5.03	105.99	111.82
1	B	97	LEU	N-CA-C	-5.02	107.55	113.97
1	B	371	VAL	N-CA-C	-5.02	106.47	113.00

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	4590	0	4527	151	0
1	B	4546	0	4488	152	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
3	B	1	0	0	0	0
All	All	9152	0	9015	295	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 16.

All (295) 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:464:GLY:O	1:B:465:PHE:CD1	1.92	1.21
1:B:188:ALA:CA	1:B:198:ARG:HD2	1.72	1.18
1:B:529:TRP:HZ3	1:B:530:TYR:CE1	1.60	1.18
1:B:188:ALA:HA	1:B:198:ARG:CD	1.73	1.16
1:A:57:ILE:HD13	1:A:67:PHE:CZ	1.87	1.10
1:A:9:ARG:HD3	1:A:213:HIS:ND1	1.69	1.08
1:B:529:TRP:CZ3	1:B:530:TYR:CE1	2.45	1.04
1:B:322:THR:OG1	1:B:323:PRO:HD3	1.59	1.03
1:A:117:LYS:HG3	1:A:118:LEU:H	1.28	0.98
1:B:11:LEU:HD21	1:B:103:ILE:HD12	1.42	0.98
1:A:322:THR:OG1	1:A:323:PRO:HD3	1.63	0.98
1:B:464:GLY:O	1:B:465:PHE:HD1	1.47	0.97
1:A:310:ASN:OD1	1:A:313:ASN:HB2	1.66	0.95
1:B:409:ASP:OD2	1:B:422:LYS:HG3	1.64	0.95
1:A:256:VAL:HG11	1:A:311:LYS:HA	1.55	0.88
1:A:97:LEU:HD22	1:B:250:LEU:HD11	1.55	0.88
1:A:400:ASP:O	1:A:404:THR:HG23	1.73	0.88
1:B:525:MET:HE1	1:B:554:GLU:O	1.74	0.87
1:A:448:ASP:OD1	1:A:506:LYS:HD3	1.74	0.87
1:A:85:VAL:CG1	1:A:88:LEU:HD11	2.06	0.85
1:A:123:TRP:CE3	1:A:502:GLU:OE2	2.29	0.85
1:B:11:LEU:HD12	1:B:20:TYR:CD2	2.13	0.84
1:B:8:ILE:O	1:B:12:LEU:HD13	1.78	0.83
1:B:465:PHE:HE2	1:B:512:LEU:HD12	1.43	0.83
1:B:370:ARG:NH2	1:B:373:TYR:HE2	1.77	0.83
1:B:427:MET:HE1	1:B:434:LEU:HD11	1.60	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:ILE:O	1:B:578:LEU:HD13	1.79	0.83
1:B:465:PHE:HE2	1:B:512:LEU:CD1	1.92	0.81
1:A:309:PHE:HA	1:A:314:MET:HE3	1.60	0.81
1:B:465:PHE:CE2	1:B:512:LEU:HD13	2.16	0.81
1:B:291:LYS:HE2	1:B:304:PHE:HB2	1.62	0.81
1:A:123:TRP:HE3	1:A:502:GLU:CD	1.88	0.81
1:B:474:ASP:OD1	1:B:475:HIS:N	2.13	0.81
1:B:507:LEU:HA	1:B:510:LEU:HD12	1.62	0.80
1:B:370:ARG:CZ	1:B:373:TYR:HE2	1.94	0.80
1:B:211:THR:HA	1:B:215:LYS:HG3	1.63	0.79
1:B:230:ARG:NH1	1:B:234:ILE:HD11	1.96	0.79
1:B:465:PHE:CE2	1:B:512:LEU:CD1	2.65	0.79
1:A:9:ARG:HD3	1:A:213:HIS:CE1	2.18	0.78
1:A:210:ARG:O	1:A:215:LYS:HG3	1.84	0.78
1:A:117:LYS:HG3	1:A:118:LEU:N	1.97	0.77
1:A:164:ALA:HB3	1:A:167:GLN:HB2	1.66	0.77
1:B:210:ARG:O	1:B:215:LYS:HE2	1.85	0.77
1:B:427:MET:HE1	1:B:434:LEU:CD1	2.13	0.77
1:B:223:GLU:HG3	1:B:224:SER:H	1.49	0.76
1:A:12:LEU:HD11	1:A:110:LEU:HD12	1.65	0.76
1:A:57:ILE:CD1	1:A:67:PHE:CZ	2.68	0.75
1:A:85:VAL:CG1	1:A:88:LEU:CD1	2.64	0.74
1:A:85:VAL:HG13	1:A:88:LEU:CD1	2.17	0.74
1:B:156:THR:OG1	1:B:159:LYS:HG2	1.87	0.74
1:A:123:TRP:HE3	1:A:502:GLU:OE2	1.69	0.74
1:A:136:LEU:HD12	1:A:151:ASP:O	1.88	0.74
1:B:223:GLU:HG3	1:B:224:SER:N	2.03	0.74
1:A:243:THR:HA	1:B:243:THR:HG23	1.69	0.74
1:B:496:GLN:O	1:B:500:LEU:HD13	1.87	0.74
1:B:11:LEU:HD12	1:B:20:TYR:CE2	2.24	0.73
1:B:271:LEU:HD13	1:B:325:ARG:HG3	1.71	0.73
1:B:302:VAL:HG12	1:B:302:VAL:O	1.88	0.73
1:A:57:ILE:CD1	1:A:67:PHE:CE1	2.72	0.72
1:B:230:ARG:HH11	1:B:234:ILE:HD11	1.55	0.72
1:A:85:VAL:HG13	1:A:88:LEU:HD11	1.69	0.72
1:B:138:LEU:HD12	1:B:168:TYR:HD2	1.53	0.72
1:A:56:LYS:HE3	1:A:222:GLU:HG2	1.72	0.71
1:A:20:TYR:CE1	1:A:94:ILE:HD13	2.27	0.70
1:B:256:VAL:HG13	1:B:264:ALA:HB3	1.74	0.70
1:B:458:LEU:HD21	1:B:507:LEU:HD11	1.74	0.69
1:B:465:PHE:CD2	1:B:512:LEU:HD13	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ARG:O	1:B:215:LYS:CE	2.41	0.69
1:B:252:LEU:O	1:B:256:VAL:HG23	1.92	0.69
1:B:370:ARG:NH2	1:B:373:TYR:CE2	2.60	0.69
1:A:243:THR:HA	1:B:243:THR:CG2	2.23	0.68
1:A:85:VAL:HG11	1:A:88:LEU:HD11	1.74	0.68
1:B:254:ILE:HD13	1:B:306:VAL:HG21	1.74	0.68
1:B:11:LEU:HD12	1:B:20:TYR:HD2	1.59	0.67
1:B:247:TYR:HD2	1:B:251:LEU:HD11	1.59	0.67
1:A:322:THR:OG1	1:A:323:PRO:CD	2.41	0.66
1:A:172:VAL:HG13	1:A:208:LEU:HD21	1.78	0.66
1:B:577:ALA:C	1:B:578:LEU:HD12	2.21	0.65
1:A:97:LEU:HD22	1:B:250:LEU:CD1	2.24	0.65
1:B:138:LEU:HD12	1:B:168:TYR:CD2	2.32	0.65
1:A:448:ASP:OD1	1:A:506:LYS:CD	2.43	0.65
1:B:51:THR:HA	1:B:219:SER:OG	1.96	0.64
1:B:464:GLY:C	1:B:465:PHE:CD1	2.75	0.64
1:B:225:ASP:OD1	1:B:226:GLN:N	2.30	0.64
1:A:59:PRO:HA	1:A:62:ARG:HB3	1.78	0.64
1:B:118:LEU:HD12	1:B:118:LEU:O	1.98	0.64
1:B:427:MET:CE	1:B:434:LEU:HD11	2.28	0.64
1:A:310:ASN:OD1	1:A:313:ASN:CB	2.43	0.63
1:B:230:ARG:NH1	1:B:234:ILE:CD1	2.61	0.63
1:B:322:THR:OG1	1:B:323:PRO:CD	2.44	0.63
1:B:11:LEU:CD1	1:B:20:TYR:CD2	2.82	0.62
1:B:172:VAL:HG13	1:B:208:LEU:HD21	1.82	0.62
1:B:576:THR:HA	1:B:579:GLN:CD	2.25	0.62
1:A:194:SER:HB2	1:A:197:GLN:HG2	1.81	0.62
1:A:527:HIS:HB3	1:A:554:GLU:OE1	2.00	0.61
1:B:271:LEU:HD13	1:B:325:ARG:CG	2.31	0.61
1:A:79:ASN:ND2	1:A:83:GLU:OE2	2.34	0.61
1:A:110:LEU:CD2	1:A:172:VAL:HG12	2.31	0.61
1:B:247:TYR:CD2	1:B:251:LEU:HD11	2.35	0.60
1:B:296:LEU:CD2	1:B:356:TYR:HA	2.31	0.60
1:B:529:TRP:HZ3	1:B:530:TYR:HE1	1.40	0.60
1:B:578:LEU:HD12	1:B:578:LEU:N	2.16	0.60
1:A:487:LEU:HD13	1:A:500:LEU:HD23	1.83	0.60
1:A:138:LEU:HD12	1:A:168:TYR:CD1	2.36	0.60
1:A:127:ASP:OD1	1:A:127:ASP:O	2.20	0.60
1:A:123:TRP:CD1	1:A:124:SER:N	2.69	0.60
1:A:256:VAL:HG13	1:A:311:LYS:HG3	1.81	0.60
1:B:254:ILE:HD13	1:B:306:VAL:CG2	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LEU:HD12	1:A:352:LEU:HD21	1.83	0.60
1:B:406:LEU:HD22	1:B:423:ILE:HG23	1.83	0.60
1:A:59:PRO:O	1:A:62:ARG:HG2	2.01	0.59
1:A:267:GLU:OE1	1:A:325:ARG:NH1	2.35	0.59
1:A:85:VAL:HG11	1:A:88:LEU:CD1	2.29	0.59
1:A:123:TRP:CZ3	1:A:502:GLU:OE2	2.55	0.59
1:B:188:ALA:HA	1:B:198:ARG:HD2	0.79	0.59
1:B:214:ASP:O	1:B:215:LYS:HG2	2.03	0.58
1:B:427:MET:CE	1:B:434:LEU:CD1	2.81	0.58
1:A:210:ARG:O	1:A:215:LYS:CG	2.50	0.58
1:A:123:TRP:CE3	1:A:502:GLU:CD	2.75	0.58
1:B:11:LEU:CD1	1:B:20:TYR:CE2	2.86	0.58
1:B:498:ASP:CG	1:B:498:ASP:O	2.47	0.58
1:A:11:LEU:HD21	1:A:103:ILE:HG12	1.86	0.58
1:B:223:GLU:CG	1:B:224:SER:H	2.16	0.57
1:B:322:THR:HG1	1:B:323:PRO:HD3	1.66	0.57
1:A:302:VAL:HG12	1:A:302:VAL:O	2.03	0.57
1:A:297:SER:HB3	1:A:316:ILE:HG22	1.87	0.57
1:A:72:GLN:HG3	1:A:73:HIS:ND1	2.20	0.57
1:A:211:THR:HA	1:A:215:LYS:HD2	1.86	0.56
1:A:12:LEU:CD1	1:A:110:LEU:HD12	2.32	0.56
1:A:254:ILE:HG21	1:A:265:ARG:HB2	1.87	0.56
1:A:11:LEU:HD22	1:A:218:ILE:HD13	1.87	0.56
1:B:370:ARG:CZ	1:B:373:TYR:CE2	2.83	0.56
1:A:526:PRO:HB2	1:A:552:LEU:HD13	1.88	0.56
1:A:18:GLN:OE1	1:A:87:GLN:HB3	2.05	0.56
1:A:57:ILE:HD11	1:A:67:PHE:CE1	2.40	0.55
1:B:271:LEU:HD22	1:B:325:ARG:HG3	1.87	0.55
1:A:59:PRO:O	1:A:62:ARG:NH2	2.36	0.55
1:A:278:VAL:HG11	1:A:333:GLN:HG2	1.89	0.55
1:A:394:ILE:HA	1:A:432:LYS:HG2	1.88	0.55
1:B:9:ARG:HG3	1:B:10:SER:N	2.22	0.55
1:B:430:ARG:O	1:B:430:ARG:HG3	2.05	0.55
1:B:466:ASP:OD2	1:B:469:ARG:CD	2.54	0.55
1:A:56:LYS:HE3	1:A:222:GLU:CG	2.36	0.55
1:A:72:GLN:HG3	1:A:73:HIS:N	2.22	0.55
1:B:302:VAL:O	1:B:302:VAL:CG1	2.55	0.55
1:A:11:LEU:HB2	1:A:218:ILE:HD13	1.88	0.54
1:B:498:ASP:HA	1:B:501:ILE:HG12	1.89	0.54
1:A:170:PHE:HE2	1:A:175:ILE:HG12	1.73	0.53
1:B:156:THR:OG1	1:B:159:LYS:CG	2.54	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ASP:OD2	1:B:192:ARG:HB3	2.08	0.53
1:A:329:LEU:O	1:A:333:GLN:HG3	2.09	0.53
1:B:214:ASP:O	1:B:215:LYS:HD3	2.09	0.53
1:A:210:ARG:O	1:A:215:LYS:CD	2.56	0.53
1:B:458:LEU:HD21	1:B:507:LEU:CD1	2.38	0.53
1:B:118:LEU:HD12	1:B:118:LEU:C	2.33	0.53
1:B:131:VAL:HG23	1:B:131:VAL:O	2.09	0.53
1:B:440:GLU:O	1:B:444:LEU:HG	2.09	0.53
1:B:159:LYS:O	1:B:162:LEU:HG	2.10	0.52
1:B:466:ASP:OD2	1:B:469:ARG:HG3	2.09	0.52
1:B:20:TYR:HE1	1:B:94:ILE:HD12	1.73	0.52
1:A:161:SER:O	1:A:161:SER:OG	2.22	0.52
1:A:387:SER:HB3	1:A:395:TRP:HE1	1.73	0.51
1:B:223:GLU:CG	1:B:224:SER:N	2.72	0.51
1:A:379:CYS:SG	1:A:420:LEU:HB2	2.50	0.51
1:B:214:ASP:O	1:B:215:LYS:CG	2.58	0.51
1:B:278:VAL:HG21	1:B:332:MET:HB2	1.92	0.51
1:A:11:LEU:HB2	1:A:218:ILE:CD1	2.41	0.51
1:A:379:CYS:SG	1:A:420:LEU:HD22	2.51	0.51
1:B:459:THR:HG23	1:B:467:PHE:CE1	2.46	0.51
1:A:385:ILE:O	1:A:389:LEU:HG	2.09	0.51
1:A:11:LEU:HD12	1:A:20:TYR:CD2	2.46	0.50
1:A:85:VAL:HG13	1:A:88:LEU:HD12	1.92	0.50
1:A:249:ASP:HA	1:A:252:LEU:HD13	1.93	0.50
1:A:132:ARG:HG2	1:A:156:THR:OG1	2.11	0.50
1:A:121:LYS:HB3	1:A:123:TRP:CZ2	2.47	0.50
1:B:507:LEU:CA	1:B:510:LEU:HD12	2.37	0.50
1:A:123:TRP:CG	1:A:124:SER:N	2.79	0.50
1:A:20:TYR:HE1	1:A:94:ILE:HD13	1.75	0.50
1:A:280:ASP:HB2	1:A:341:ASN:OD1	2.11	0.50
1:A:314:MET:CE	1:A:317:LEU:HD22	2.41	0.50
1:B:296:LEU:HD23	1:B:356:TYR:HA	1.94	0.50
1:B:578:LEU:N	1:B:578:LEU:CD1	2.74	0.50
1:A:117:LYS:CG	1:A:118:LEU:H	2.03	0.50
1:B:557:ASN:OD1	1:B:558:GLN:HG2	2.12	0.50
1:A:253:SER:C	1:A:255:ALA:N	2.69	0.49
1:A:382:ASN:ND2	1:A:386:ARG:NH1	2.59	0.49
1:A:527:HIS:O	1:A:527:HIS:ND1	2.45	0.49
1:B:419:PRO:O	1:B:423:ILE:HG12	2.12	0.49
1:A:385:ILE:HG21	1:A:460:LEU:HB2	1.94	0.49
1:A:194:SER:H	1:A:197:GLN:CG	2.24	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:VAL:HG12	1:B:198:ARG:HG3	1.94	0.49
1:A:56:LYS:CE	1:A:222:GLU:HG2	2.41	0.49
1:A:371:VAL:HG12	1:A:371:VAL:O	2.11	0.49
1:B:427:MET:HE1	1:B:434:LEU:HD12	1.93	0.49
1:A:189:ASP:OD1	1:A:189:ASP:O	2.31	0.49
1:A:251:LEU:HA	1:A:254:ILE:HG12	1.95	0.49
1:A:275:MET:HE2	1:A:284:VAL:HG21	1.94	0.49
1:A:85:VAL:CG1	1:A:88:LEU:HD12	2.43	0.48
1:B:180:GLU:O	1:B:184:ILE:HG12	2.13	0.48
1:B:8:ILE:O	1:B:12:LEU:CD1	2.56	0.48
1:B:247:TYR:O	1:B:250:LEU:HB3	2.13	0.48
1:A:66:GLN:OE1	1:B:258:GLN:HA	2.12	0.48
1:A:104:THR:O	1:A:108:ILE:HG12	2.14	0.48
1:B:529:TRP:CZ3	1:B:530:TYR:CD1	2.98	0.48
1:B:576:THR:HA	1:B:579:GLN:HG3	1.94	0.48
1:A:430:ARG:HG3	1:A:430:ARG:O	2.13	0.48
1:B:296:LEU:HD12	1:B:324:ILE:HG23	1.95	0.48
1:B:210:ARG:O	1:B:215:LYS:CG	2.62	0.48
1:A:324:ILE:O	1:A:325:ARG:C	2.57	0.48
1:B:214:ASP:O	1:B:215:LYS:CD	2.62	0.47
1:A:11:LEU:HD22	1:A:218:ILE:CD1	2.44	0.47
1:B:462:PHE:HB3	1:B:465:PHE:CZ	2.50	0.47
1:A:256:VAL:CG1	1:A:311:LYS:HG3	2.45	0.47
1:A:288:LEU:CD1	1:A:352:LEU:HD21	2.45	0.47
1:A:483:THR:OG1	1:A:486:LYS:CB	2.63	0.47
1:A:335:LEU:HD11	1:A:351:ILE:HG12	1.96	0.46
1:B:40:PHE:O	1:B:44:LEU:HD13	2.15	0.46
1:A:56:LYS:CG	1:A:222:GLU:HG2	2.45	0.46
1:B:429:GLN:C	1:B:431:GLY:H	2.23	0.46
1:A:138:LEU:HD12	1:A:168:TYR:HD1	1.78	0.46
1:B:188:ALA:CB	1:B:198:ARG:HH11	2.29	0.46
1:B:328:LEU:HD23	1:B:355:ALA:HB1	1.96	0.46
1:A:483:THR:OG1	1:A:486:LYS:HB2	2.16	0.46
1:A:59:PRO:HB3	1:A:62:ARG:HD3	1.98	0.46
1:B:211:THR:HA	1:B:215:LYS:CG	2.42	0.46
1:A:468:SER:OG	1:A:469:ARG:N	2.49	0.45
1:B:188:ALA:HB1	1:B:198:ARG:NH1	2.32	0.45
1:B:210:ARG:O	1:B:215:LYS:HG2	2.16	0.45
1:A:451:ASN:HD21	1:A:453:ARG:HH11	1.63	0.45
1:A:36:ILE:HD12	1:A:105:ALA:CB	2.46	0.45
1:B:99:GLY:O	1:B:103:ILE:HG12	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:ASP:OD2	1:B:469:ARG:NE	2.48	0.45
1:A:302:VAL:O	1:A:302:VAL:CG1	2.65	0.45
1:B:575:ARG:O	1:B:579:GLN:HG3	2.17	0.44
1:A:124:SER:OG	1:A:126:ASP:O	2.35	0.44
1:B:214:ASP:C	1:B:215:LYS:HG2	2.43	0.44
1:B:297:SER:HB2	1:B:299:ILE:HG12	1.99	0.44
1:B:465:PHE:HB2	1:B:467:PHE:CE1	2.53	0.44
1:A:72:GLN:HG3	1:A:73:HIS:H	1.83	0.43
1:B:7:THR:HG22	1:B:215:LYS:O	2.19	0.43
1:A:133:ARG:HE	1:A:171:ARG:HD2	1.83	0.43
1:A:540:ARG:O	1:A:541:GLN:C	2.61	0.43
1:B:56:LYS:HG2	1:B:94:ILE:HG12	2.01	0.43
1:B:261:SER:C	1:B:263:ASP:H	2.27	0.43
1:B:529:TRP:CE3	1:B:530:TYR:CE1	3.03	0.43
1:A:75:HIS:O	1:A:76:GLU:C	2.60	0.43
1:A:176:MET:HE3	1:A:176:MET:HB3	1.77	0.43
1:A:402:LEU:HD11	1:A:427:MET:HG2	2.01	0.43
1:A:278:VAL:CG1	1:A:333:GLN:HG2	2.48	0.43
1:A:303:GLY:C	1:A:305:LYS:H	2.26	0.43
1:B:275:MET:O	1:B:278:VAL:HG23	2.19	0.43
1:A:97:LEU:CD2	1:B:250:LEU:HD11	2.39	0.43
1:B:576:THR:HA	1:B:579:GLN:CG	2.48	0.43
1:A:507:LEU:HG	1:A:570:LEU:HD13	2.01	0.42
1:A:65:TYR:HB2	1:A:67:PHE:CZ	2.54	0.42
1:B:329:LEU:O	1:B:333:GLN:HG3	2.19	0.42
1:B:459:THR:HG23	1:B:467:PHE:CZ	2.54	0.42
1:B:552:LEU:HD23	1:B:552:LEU:HA	1.92	0.42
1:A:53:LEU:H	1:A:98:ASP:HB3	1.84	0.42
1:A:56:LYS:HE3	1:A:222:GLU:CD	2.45	0.42
1:B:487:LEU:HD23	1:B:556:LEU:HD23	2.00	0.42
1:B:443:GLU:O	1:B:446:GLN:HG3	2.19	0.42
1:A:136:LEU:HD13	1:A:152:PHE:CE1	2.55	0.42
1:A:253:SER:O	1:A:254:ILE:C	2.60	0.42
1:A:513:LEU:HA	1:A:513:LEU:HD12	1.80	0.42
1:A:552:LEU:HD23	1:A:552:LEU:HA	1.87	0.42
1:A:483:THR:O	1:A:484:ARG:C	2.63	0.42
1:A:525:MET:HE3	1:A:525:MET:HB3	1.60	0.42
1:B:328:LEU:O	1:B:331:SER:HB2	2.20	0.42
1:A:57:ILE:HD13	1:A:67:PHE:HZ	1.67	0.41
1:A:194:SER:H	1:A:197:GLN:HG3	1.84	0.41
1:A:243:THR:HB	1:B:243:THR:OG1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ASN:HB3	1:B:237:ARG:HH12	1.84	0.41
1:B:496:GLN:O	1:B:500:LEU:CD1	2.65	0.41
1:A:251:LEU:C	1:A:253:SER:N	2.75	0.41
1:A:291:LYS:HE2	1:A:302:VAL:HG12	2.02	0.41
1:A:313:ASN:C	1:A:315:ALA:N	2.79	0.41
1:A:443:GLU:O	1:A:446:GLN:HG3	2.20	0.41
1:B:529:TRP:CE3	1:B:530:TYR:CD1	3.08	0.41
1:B:444:LEU:O	1:B:447:LEU:HG	2.20	0.41
1:A:75:HIS:CE1	1:A:77:ARG:HB3	2.55	0.41
1:B:328:LEU:HD23	1:B:355:ALA:CB	2.51	0.41
1:B:556:LEU:HD12	1:B:556:LEU:HA	1.94	0.41
1:A:243:THR:HG23	1:A:243:THR:O	2.20	0.41
1:A:413:SER:HB3	1:A:419:PRO:HB3	2.03	0.41
1:B:336:ALA:C	1:B:339:GLY:H	2.29	0.41
1:A:136:LEU:HD13	1:A:152:PHE:CD1	2.55	0.41
1:B:548:ALA:HB3	1:B:566:ARG:NH1	2.36	0.41
1:A:126:ASP:C	1:A:128:ALA:H	2.29	0.40
1:B:430:ARG:O	1:B:430:ARG:CG	2.69	0.40
1:A:228:LEU:HD21	1:B:250:LEU:HD21	2.03	0.40
1:A:313:ASN:C	1:A:315:ALA:H	2.29	0.40
1:B:71:MET:HE1	1:B:79:ASN:HB3	2.04	0.40
1:A:110:LEU:HD23	1:A:172:VAL:HG12	2.04	0.40
1:B:22:LEU:HD23	1:B:22:LEU:HA	1.90	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	553/587 (94%)	518 (94%)	35 (6%)	0	100	100
1	B	545/587 (93%)	522 (96%)	23 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1098/1174 (94%)	1040 (95%)	58 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	494/516 (96%)	491 (99%)	3 (1%)	78	89
1	B	490/516 (95%)	485 (99%)	5 (1%)	68	83
All	All	984/1032 (95%)	976 (99%)	8 (1%)	73	86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	TYR
1	A	525	MET
1	A	566	ARG
1	B	123	TRP
1	B	247	TYR
1	B	295	MET
1	B	427	MET
1	B	566	ARG

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

Mol	Chain	Res	Type
1	A	79	ASN
1	A	333	GLN
1	A	412	GLN
1	A	518	ASN
1	B	18	GLN
1	B	69	GLN
1	B	73	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	101	GLN
1	B	269	HIS
1	B	360	HIS
1	B	412	GLN
1	B	496	GLN
1	B	509	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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	601	-	4,4,4	0.45	0	6,6,6	0.10	0
2	SO4	B	602	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	B	601	-	4,4,4	0.47	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	563/587 (95%)	0.56	42 (7%)	20 14	69, 97, 129, 146	0
1	B	557/587 (94%)	0.52	44 (7%)	18 14	64, 92, 123, 141	0
All	All	1120/1174 (95%)	0.54	86 (7%)	19 14	64, 95, 126, 146	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	ILE	7.5
1	B	24	ALA	5.7
1	A	528	GLU	5.1
1	B	526	PRO	5.0
1	B	529	TRP	4.9
1	A	268	ILE	4.8
1	A	112	GLY	4.5
1	A	267	GLU	4.5
1	B	20	TYR	4.4
1	A	473	VAL	4.0
1	B	514	GLU	3.9
1	A	321	TRP	3.8
1	A	266	GLU	3.8
1	A	490	VAL	3.7
1	A	330	LEU	3.7
1	B	54	PHE	3.7
1	A	274	GLU	3.7
1	B	144	LEU	3.6
1	B	130	PRO	3.6
1	B	580	PRO	3.6
1	B	473	VAL	3.5
1	A	579	GLN	3.4
1	A	290	LEU	3.3
1	A	304	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	489	LYS	3.3
1	A	554	GLU	3.2
1	B	481	LEU	3.2
1	A	269	HIS	3.1
1	A	326	ASP	3.1
1	A	485	ASN	3.1
1	B	476	ILE	3.1
1	A	212	ILE	3.1
1	B	23	PRO	3.1
1	B	528	GLU	3.0
1	A	325	ARG	2.9
1	B	530	TYR	2.9
1	B	571	LEU	2.9
1	A	144	LEU	2.8
1	A	275	MET	2.8
1	A	265	ARG	2.8
1	A	486	LYS	2.8
1	A	123	TRP	2.8
1	B	532	GLN	2.7
1	B	9	ARG	2.7
1	A	25	ILE	2.7
1	A	271	LEU	2.7
1	A	481	LEU	2.7
1	B	438	PRO	2.7
1	B	17	GLU	2.7
1	B	525	MET	2.6
1	B	449	TYR	2.6
1	A	337	SER	2.5
1	B	280	ASP	2.5
1	A	449	TYR	2.5
1	B	225	ASP	2.5
1	B	53	LEU	2.5
1	B	94	ILE	2.5
1	B	11	LEU	2.4
1	B	343	GLN	2.4
1	A	117	LYS	2.4
1	A	483	THR	2.4
1	B	22	LEU	2.4
1	A	273	ASP	2.3
1	A	527	HIS	2.3
1	B	218	ILE	2.3
1	A	244	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	244	THR	2.3
1	B	219	SER	2.3
1	B	167	GLN	2.2
1	B	524	LYS	2.2
1	A	520	GLN	2.2
1	B	212	ILE	2.2
1	B	465	PHE	2.2
1	B	262	LEU	2.2
1	B	100	GLN	2.2
1	B	511	GLN	2.2
1	B	93	PHE	2.2
1	A	333	GLN	2.2
1	A	484	ARG	2.1
1	A	252	LEU	2.1
1	B	44	LEU	2.1
1	B	162	LEU	2.1
1	A	119	THR	2.1
1	B	474	ASP	2.1
1	A	488	ALA	2.1
1	A	282	PHE	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(Å ²)	Q<0.9
2	SO4	B	602	5/5	0.65	0.07	120,123,133,143	0
2	SO4	A	601	5/5	0.82	0.10	90,103,109,114	0
3	CL	B	603	1/1	0.85	0.19	107,107,107,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	601	5/5	0.86	0.10	90,99,108,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.