



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:55 am BST

PDB ID : 6OAO
Title : Structure of DBP in complex with human neutralizing antibody 092096
Authors : Urusova, D.; Tolia, N.H.
Deposited on : 2019-03-18
Resolution : 3.50 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

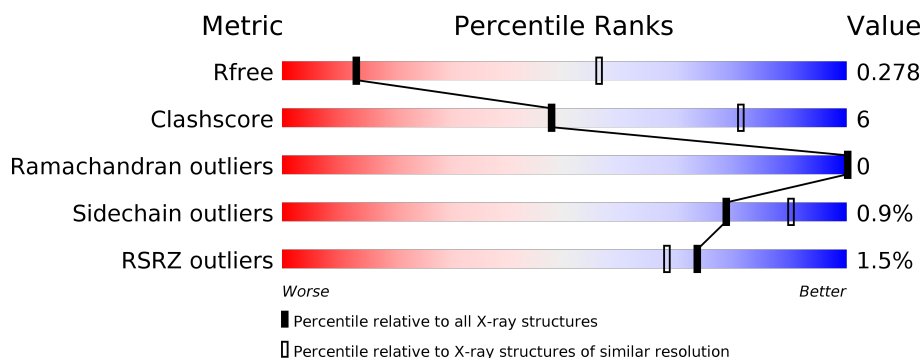
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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	315	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>
1	C	315	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>9%</div> </div> </div>
1	E	315	<div> <div></div> <div> <div></div> <div>78%</div> <div>13%</div> <div>10%</div> </div> </div>
1	G	315	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>10%</div> </div> </div>
1	I	315	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>6%</div> <div>9%</div> </div> </div>
1	K	315	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>10%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	251	<div><div><div></div><div></div><div></div></div><div>3%76%14%10%</div></div>
2	D	251	<div><div><div></div><div></div><div></div></div><div>%77%13%10%</div></div>
2	F	251	<div><div><div></div><div></div><div></div></div><div>3%80%11%9%</div></div>
2	H	251	<div><div><div></div><div></div><div></div></div><div>2%78%12%9%</div></div>
2	J	251	<div><div><div></div><div></div><div></div></div><div>79%12%9%</div></div>
2	L	251	<div><div><div></div><div></div><div></div></div><div>%82%8%10%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24648 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 Duffy binding surface protein region II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2374	1507	418	432	17			
1	C	288	Total	C	N	O	S	0	0	0
			2405	1523	424	441	17			
1	E	285	Total	C	N	O	S	0	0	0
			2383	1513	420	433	17			
1	G	284	Total	C	N	O	S	0	0	0
			2374	1507	418	432	17			
1	I	287	Total	C	N	O	S	0	0	0
			2397	1519	423	438	17			
1	K	285	Total	C	N	O	S	0	0	0
			2383	1513	420	433	17			

- Molecule 2 is a protein called Antibody 092096 single chain variable fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1712	1065	288	351	8			
2	D	227	Total	C	N	O	S	0	0	0
			1712	1065	288	351	8			
2	F	229	Total	C	N	O	S	0	0	0
			1725	1072	290	355	8			
2	H	229	Total	C	N	O	S	0	0	0
			1728	1074	292	354	8			
2	J	228	Total	C	N	O	S	0	0	0
			1718	1068	289	353	8			
2	L	227	Total	C	N	O	S	0	0	0
			1712	1065	288	351	8			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		

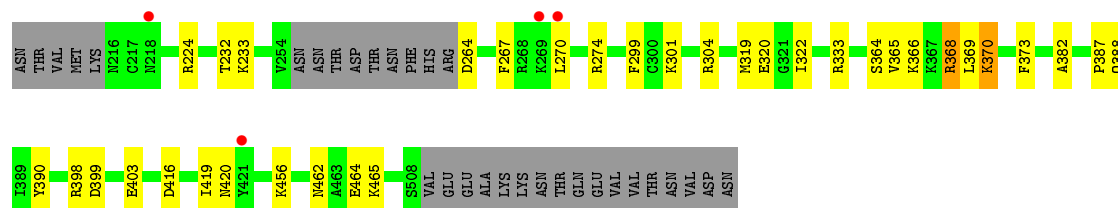
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	E	3	Total	O	0	0
			3	3		
4	F	2	Total	O	0	0
			2	2		
4	G	1	Total	O	0	0
			1	1		
4	I	2	Total	O	0	0
			2	2		
4	K	4	Total	O	0	0
			4	4		
4	L	1	Total	O	0	0
			1	1		

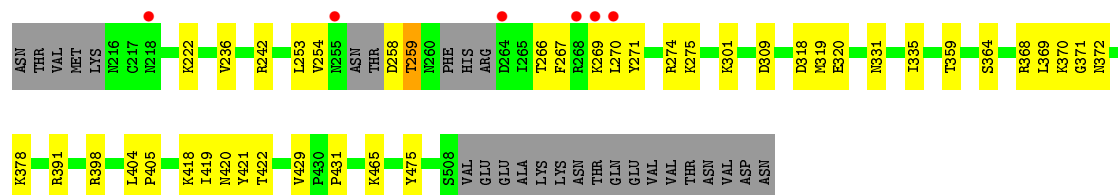
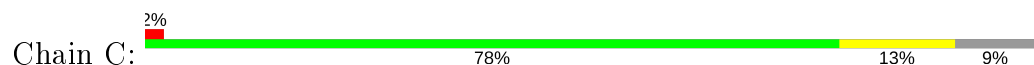
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

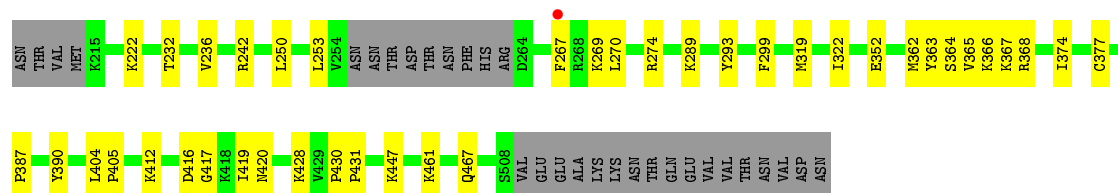
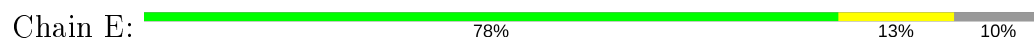
- Molecule 1: Duffy binding surface protein region II



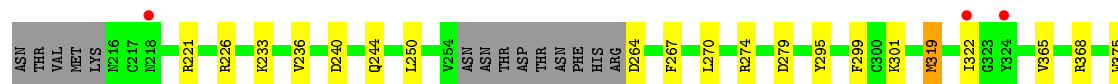
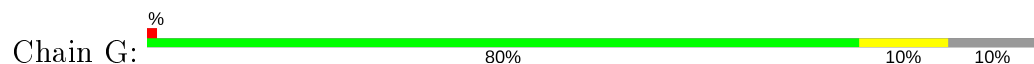
- Molecule 1: Duffy binding surface protein region II



- Molecule 1: Duffy binding surface protein region II



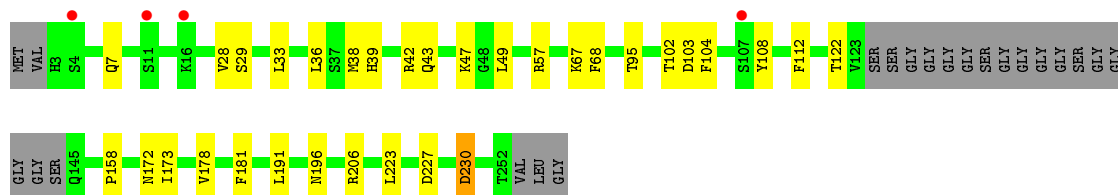
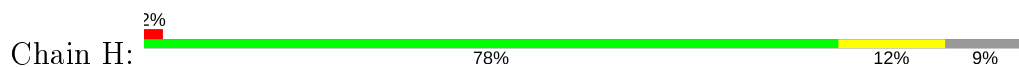
- Molecule 1: Duffy binding surface protein region II



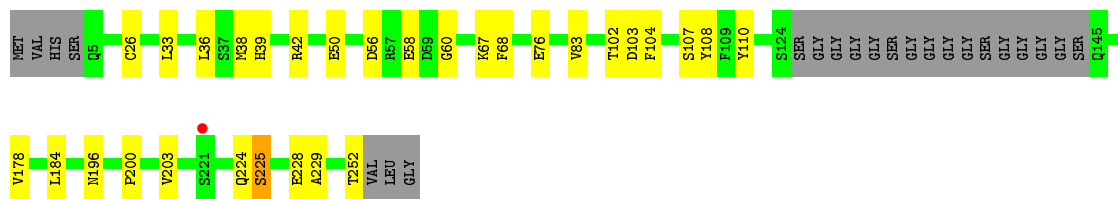
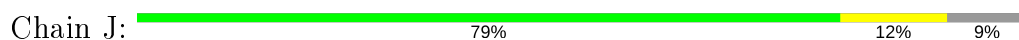




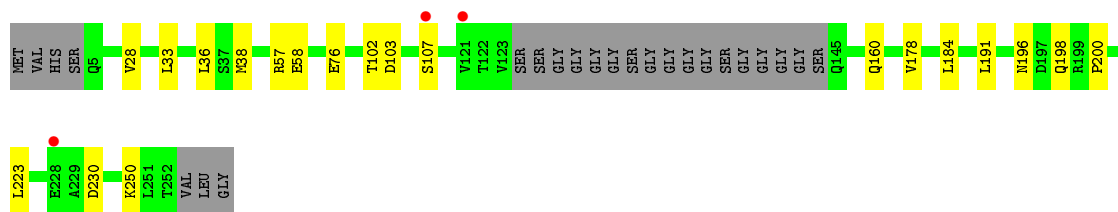
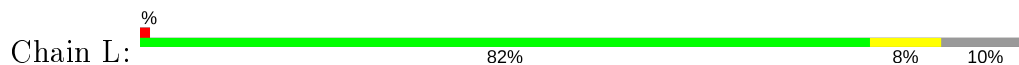
- Molecule 2: Antibody 092096 single chain variable fragment



- Molecule 2: Antibody 092096 single chain variable fragment



- Molecule 2: Antibody 092096 single chain variable fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.66 Å 89.56 Å 193.71 Å 90.00° 108.05° 90.00°	Depositor
Resolution (Å)	19.97 – 3.50 19.97 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.97-3.50) 99.7 (19.97-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.52 Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.237 , 0.279 0.240 , 0.278	Depositor DCC
R_{free} test set	2787 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 17.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.073 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	24648	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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 [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	0.34	0/2420	0.46	0/3254
1	C	0.35	0/2450	0.47	0/3294
1	E	0.37	0/2429	0.48	0/3265
1	G	0.33	0/2420	0.47	0/3254
1	I	0.32	0/2443	0.47	0/3286
1	K	0.38	0/2429	0.49	0/3265
2	B	0.37	0/1749	0.57	0/2371
2	D	0.41	0/1749	0.59	0/2371
2	F	0.49	1/1762 (0.1%)	0.61	0/2389
2	H	0.36	0/1766	0.56	0/2394
2	J	0.39	0/1755	0.54	0/2379
2	L	0.40	0/1749	0.56	0/2371
All	All	0.37	1/25121 (0.0%)	0.52	0/33893

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	69	GLN	C-N	-5.06	1.24	1.33

There are no bond angle outliers.

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	2374	0	2371	32	0
1	C	2405	0	2393	37	0
1	E	2383	0	2384	35	0
1	G	2374	0	2371	21	0
1	I	2397	0	2390	13	0
1	K	2383	0	2384	31	0
2	B	1712	0	1608	32	0
2	D	1712	0	1608	26	0
2	F	1725	0	1622	23	0
2	H	1728	0	1620	23	0
2	J	1718	0	1613	24	0
2	L	1712	0	1608	21	0
3	E	5	0	0	1	0
4	A	5	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	3	0	0	1	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
4	I	2	0	0	0	0
4	K	4	0	0	0	0
4	L	1	0	0	0	0
All	All	24648	0	23972	294	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 6.

All (294) 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:E:362:MET:HE3	1:E:377:CYS:HB2	1.39	1.02
1:E:364:SER:O	1:E:368:ARG:HG3	1.70	0.91
2:L:178:VAL:HB	2:L:196:ASN:ND2	1.88	0.89
1:E:362:MET:HE3	1:E:377:CYS:CB	2.07	0.84
1:E:363:TYR:HD1	2:F:105:GLY:O	1.59	0.83
2:J:102:THR:HG22	2:J:104:PHE:H	1.49	0.77
1:K:319:MET:HE3	1:K:456:LYS:HE2	1.67	0.76
2:B:178:VAL:N	2:B:196:ASN:OD1	2.20	0.75
2:D:38:MET:SD	2:D:102:THR:OG1	2.44	0.74
2:L:178:VAL:HB	2:L:196:ASN:HD22	1.52	0.74
2:H:230:ASP:N	2:H:230:ASP:OD1	2.21	0.73
2:F:177:PRO:HA	2:F:196:ASN:HD21	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:178:VAL:CB	2:L:196:ASN:ND2	2.53	0.72
1:E:366:LYS:HD3	2:F:105:GLY:HA2	1.70	0.72
2:B:39:HIS:HB2	2:B:112:PHE:HE1	1.57	0.69
2:L:178:VAL:CB	2:L:196:ASN:HD21	2.06	0.69
2:J:36:LEU:HD23	2:J:102:THR:HG21	1.74	0.68
2:D:39:HIS:HE2	2:D:110:TYR:HE2	1.42	0.68
2:D:102:THR:HG22	2:D:104:PHE:H	1.59	0.67
1:E:416:ASP:OD1	1:E:417:GLY:N	2.28	0.67
2:D:56:ASP:O	2:D:60:GLY:N	2.27	0.67
2:F:28:VAL:CG1	2:F:38:MET:HE3	2.25	0.66
2:L:178:VAL:H	2:L:196:ASN:ND2	1.93	0.66
2:L:178:VAL:HG23	2:L:196:ASN:HD21	1.60	0.66
1:E:362:MET:HE1	1:E:377:CYS:SG	2.35	0.66
2:J:38:MET:SD	2:J:102:THR:OG1	2.54	0.66
2:L:191:LEU:HD12	2:L:200:PRO:HG3	1.78	0.65
1:A:232:THR:HG23	1:A:233:LYS:H	1.61	0.64
2:H:178:VAL:N	2:H:196:ASN:OD1	2.25	0.64
1:E:412:LYS:NZ	4:E:701:HOH:O	2.31	0.63
1:C:253:LEU:HD21	1:C:275:LYS:HG3	1.80	0.63
2:J:42:ARG:NH2	2:J:50:GLU:OE1	2.32	0.62
1:E:362:MET:CE	1:E:377:CYS:SG	2.87	0.62
1:C:270:LEU:HD23	1:C:270:LEU:O	2.00	0.62
2:L:178:VAL:CG2	2:L:196:ASN:HD21	2.13	0.61
2:D:178:VAL:N	2:D:196:ASN:OD1	2.30	0.61
1:K:319:MET:HG3	1:K:388:GLN:OE1	2.00	0.61
1:C:421:TYR:HB2	1:K:369:LEU:HD21	1.82	0.61
1:C:254:VAL:O	1:C:258:ASP:HB3	2.00	0.61
2:B:28:VAL:CG1	2:B:38:MET:CE	2.79	0.60
2:L:178:VAL:N	2:L:196:ASN:HD21	2.00	0.59
2:B:28:VAL:CG1	2:B:38:MET:HE1	2.32	0.59
2:D:55:PHE:CE1	2:D:60:GLY:HA2	2.37	0.59
2:D:60:GLY:O	2:D:61:GLU:C	2.40	0.59
1:A:320:GLU:HG2	1:A:322:ILE:HG22	1.85	0.59
1:E:232:THR:HG21	1:E:322:ILE:HD13	1.85	0.59
1:A:224:ARG:HE	1:A:403:GLU:HG3	1.67	0.58
2:J:178:VAL:N	2:J:196:ASN:OD1	2.35	0.58
2:H:206:ARG:NH1	2:H:227:ASP:OD2	2.36	0.58
2:B:230:ASP:OD1	2:B:230:ASP:N	2.36	0.57
1:E:236:VAL:HG21	1:E:319:MET:HE3	1.86	0.57
1:E:419:ILE:HG23	1:E:420:ASN:H	1.70	0.57
1:C:369:LEU:HD11	1:C:372:ASN:HB2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:LEU:HD22	2:H:38:MET:HE2	1.85	0.57
2:B:33:LEU:HA	2:B:36:LEU:HD13	1.85	0.57
1:C:419:ILE:HG23	1:C:420:ASN:H	1.69	0.57
2:F:178:VAL:HB	2:F:196:ASN:OD1	2.04	0.57
1:G:295:TYR:CG	1:G:376:ILE:HD12	2.40	0.57
1:K:317:THR:O	1:K:317:THR:HG22	2.05	0.57
1:A:419:ILE:HG23	1:A:420:ASN:H	1.69	0.56
1:K:419:ILE:HG23	1:K:420:ASN:H	1.69	0.56
1:C:369:LEU:CD1	1:C:372:ASN:HB2	2.35	0.56
2:J:228:GLU:OE1	2:J:252:THR:HA	2.04	0.56
1:K:233:LYS:HE3	1:K:320:GLU:O	2.05	0.56
2:H:33:LEU:O	2:H:57:ARG:NH1	2.39	0.56
1:G:419:ILE:HG23	1:G:420:ASN:H	1.70	0.56
2:B:158:PRO:HA	2:B:223:LEU:O	2.05	0.56
1:A:232:THR:HG23	1:A:233:LYS:N	2.20	0.56
2:L:178:VAL:N	2:L:196:ASN:ND2	2.54	0.56
1:A:319:MET:HG3	1:A:388:GLN:OE1	2.06	0.56
1:C:236:VAL:HG21	1:C:319:MET:CE	2.36	0.56
1:A:462:ASN:HB3	1:E:374:ILE:HG23	1.88	0.55
2:F:177:PRO:HA	2:F:196:ASN:ND2	2.22	0.55
1:K:233:LYS:CE	1:K:320:GLU:O	2.55	0.54
2:F:191:LEU:HD12	2:F:200:PRO:HG3	1.88	0.54
1:I:419:ILE:HG23	1:I:420:ASN:H	1.70	0.54
1:E:270:LEU:HD23	1:E:274:ARG:HG3	1.89	0.54
1:C:254:VAL:HB	1:C:331:ASN:ND2	2.23	0.54
1:K:368:ARG:HH11	1:K:368:ARG:HG3	1.73	0.54
1:A:369:LEU:HD11	1:A:373:PHE:HA	1.90	0.54
1:E:387:PRO:HB2	1:E:390:TYR:CD1	2.43	0.54
2:F:193:ILE:HD12	2:F:218:LEU:HD13	1.91	0.53
2:B:237:ASP:OD2	2:B:240:LEU:N	2.42	0.53
2:D:33:LEU:HD23	2:D:57:ARG:HH12	1.72	0.53
2:J:56:ASP:O	2:J:60:GLY:N	2.41	0.53
1:G:240:ASP:OD2	1:G:244:GLN:NE2	2.41	0.53
2:J:26:CYS:SG	2:J:38:MET:HE1	2.49	0.53
1:A:319:MET:HE3	1:A:456:LYS:HE2	1.90	0.52
2:L:28:VAL:CG1	2:L:38:MET:HE3	2.39	0.52
1:C:378:LYS:HG3	1:E:467:GLN:HB3	1.91	0.52
1:C:253:LEU:CD2	1:C:275:LYS:HG3	2.40	0.52
1:C:309:ASP:OD1	1:C:391:ARG:NH2	2.42	0.51
2:H:38:MET:SD	2:H:102:THR:OG1	2.68	0.51
2:J:102:THR:HG22	2:J:104:PHE:N	2.21	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:58:GLU:HB2	2:L:107:SER:CB	2.40	0.51
1:I:236:VAL:HG21	1:I:319:MET:HE3	1.93	0.51
1:G:368:ARG:HH11	1:G:368:ARG:HG3	1.76	0.51
1:K:224:ARG:O	1:K:224:ARG:HG2	2.11	0.51
2:B:33:LEU:HD23	2:B:33:LEU:O	2.10	0.51
2:H:104:PHE:CD1	2:H:104:PHE:O	2.63	0.50
2:B:52:MET:O	2:B:65:ALA:N	2.41	0.50
1:A:464:GLU:O	1:A:465:LYS:HG2	2.12	0.50
1:A:387:PRO:HB2	1:A:390:TYR:CD1	2.47	0.50
1:A:369:LEU:HD12	1:A:369:LEU:O	2.12	0.50
2:J:104:PHE:CD1	2:J:104:PHE:O	2.65	0.49
1:C:236:VAL:HG21	1:C:319:MET:HE3	1.93	0.49
2:J:184:LEU:HG	2:J:229:ALA:HB2	1.95	0.49
1:C:368:ARG:HD3	1:K:421:TYR:OH	2.12	0.49
2:D:16:LYS:HE2	2:D:21:SER:O	2.12	0.49
1:A:270:LEU:O	1:A:274:ARG:HG3	2.12	0.49
1:K:419:ILE:HD13	1:K:428:LYS:HD3	1.94	0.49
2:F:195:SER:O	2:F:196:ASN:HB2	2.13	0.49
1:C:378:LYS:NZ	1:E:461:LYS:O	2.45	0.49
2:H:33:LEU:HD23	2:H:57:ARG:HH12	1.77	0.49
2:D:206:ARG:CZ	2:D:224:GLN:HG3	2.43	0.49
1:A:224:ARG:HH21	1:A:399:ASP:HA	1.78	0.48
1:C:359:THR:HG22	2:D:107:SER:OG	2.12	0.48
2:H:181:PHE:HE1	2:H:191:LEU:HD23	1.77	0.48
1:G:274:ARG:NH2	2:H:108:TYR:O	2.46	0.48
1:E:447:LYS:NZ	3:E:601:SO4:O3	2.32	0.48
1:I:378:LYS:HG3	1:K:467:GLN:HB2	1.95	0.48
2:D:33:LEU:HD23	2:D:33:LEU:O	2.13	0.48
1:A:465:LYS:O	1:A:465:LYS:HG3	2.13	0.48
2:D:28:VAL:CG1	2:D:38:MET:HE3	2.44	0.48
2:J:36:LEU:HB3	2:J:102:THR:HG21	1.94	0.48
1:E:467:GLN:O	1:E:467:GLN:HG3	2.14	0.47
1:G:295:TYR:CD2	1:G:376:ILE:HD12	2.50	0.47
1:A:301:LYS:HE3	1:A:398:ARG:HE	1.78	0.47
2:J:26:CYS:SG	2:J:38:MET:CE	3.03	0.47
2:B:28:VAL:HG11	2:B:38:MET:CE	2.43	0.47
1:A:366:LYS:HD3	2:B:105:GLY:HA2	1.96	0.47
1:I:372:ASN:O	1:I:372:ASN:ND2	2.46	0.47
2:J:33:LEU:O	2:J:33:LEU:HD23	2.15	0.47
1:I:378:LYS:NZ	1:K:461:LYS:O	2.40	0.47
1:E:419:ILE:HD13	1:E:428:LYS:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:221:ARG:CZ	1:G:226:ARG:HH11	2.27	0.47
1:K:389:ILE:HG23	1:K:390:TYR:HD1	1.79	0.47
2:D:228:GLU:OE1	2:D:252:THR:HG22	2.14	0.47
2:B:38:MET:HG3	2:B:83:VAL:HG21	1.96	0.47
2:D:172:ASN:OD1	2:D:173:ILE:N	2.48	0.47
2:D:181:PHE:HE1	2:D:191:LEU:HD23	1.79	0.47
1:E:362:MET:HE3	1:E:377:CYS:SG	2.54	0.47
2:H:42:ARG:HH21	2:H:68:PHE:HZ	1.63	0.47
2:B:36:LEU:HD12	2:B:36:LEU:N	2.30	0.47
2:D:36:LEU:HB3	2:D:102:THR:HG21	1.96	0.47
2:D:191:LEU:HD12	2:D:200:PRO:HG3	1.97	0.47
1:A:232:THR:CG2	1:A:233:LYS:H	2.27	0.46
1:E:419:ILE:HG23	1:E:420:ASN:N	2.30	0.46
1:G:250:LEU:N	1:G:279:ASP:OD2	2.46	0.46
2:L:36:LEU:HB3	2:L:102:THR:HG21	1.97	0.46
1:A:333:ARG:NH2	2:F:77:ASP:OD1	2.47	0.46
1:A:224:ARG:HD3	1:A:403:GLU:HG2	1.96	0.46
2:B:36:LEU:HD12	2:B:36:LEU:H	1.80	0.46
1:A:299:PHE:CZ	1:A:365:VAL:HG21	2.50	0.46
1:A:419:ILE:HG23	1:A:420:ASN:N	2.30	0.46
2:B:223:LEU:HD11	2:B:227:ASP:CB	2.45	0.46
2:F:59:ASP:OD1	2:F:59:ASP:O	2.34	0.46
1:G:233:LYS:HG3	1:G:322:ILE:HD11	1.96	0.46
1:G:375:TRP:CZ2	1:I:465:LYS:HD3	2.51	0.46
2:B:223:LEU:HD11	2:B:227:ASP:HB3	1.96	0.46
2:H:39:HIS:HB2	2:H:112:PHE:HE2	1.81	0.46
2:J:200:PRO:HD2	2:J:203:VAL:HG21	1.96	0.46
2:J:67:LYS:O	2:J:68:PHE:HD1	1.98	0.46
1:C:266:THR:O	1:C:269:LYS:O	2.34	0.46
1:G:270:LEU:O	1:G:274:ARG:HG3	2.16	0.46
1:K:419:ILE:HG23	1:K:420:ASN:N	2.31	0.46
1:E:289:LYS:HG2	1:E:293:TYR:CZ	2.51	0.46
2:F:196:ASN:OD1	2:F:211:LYS:HD3	2.16	0.46
2:J:33:LEU:HD22	2:J:76:GLU:OE2	2.16	0.46
1:C:254:VAL:CG1	1:C:331:ASN:HD21	2.29	0.45
1:C:301:LYS:HE3	1:C:398:ARG:HE	1.81	0.45
1:I:359:THR:HG21	2:J:58:GLU:OE1	2.16	0.45
2:B:39:HIS:CD2	2:B:54:GLY:HA3	2.51	0.45
2:F:28:VAL:HG12	2:F:38:MET:HE3	1.96	0.45
2:B:33:LEU:HA	2:B:36:LEU:CD1	2.47	0.45
1:G:404:LEU:HB3	1:G:405:PRO:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:THR:HG22	2:D:103:ASP:N	2.30	0.45
2:H:158:PRO:HA	2:H:223:LEU:O	2.17	0.45
2:H:43:GLN:HB2	2:H:49:LEU:HD23	1.99	0.45
2:J:33:LEU:HD11	2:J:83:VAL:HG23	1.98	0.45
1:K:364:SER:HB2	1:K:368:ARG:NH1	2.31	0.45
1:I:270:LEU:O	1:I:274:ARG:HG3	2.17	0.45
1:G:462:ASN:HB3	1:K:374:ILE:HG23	1.98	0.45
1:K:441:GLN:O	1:K:445:ARG:HG3	2.17	0.45
1:G:301:LYS:HE3	1:G:398:ARG:HE	1.82	0.45
2:B:28:VAL:CG1	2:B:38:MET:HE3	2.46	0.44
1:A:224:ARG:HD3	1:A:403:GLU:CG	2.48	0.44
1:C:242:ARG:HH21	1:C:318:ASP:CG	2.21	0.44
2:H:102:THR:HG22	2:H:103:ASP:N	2.33	0.44
1:C:259:THR:OG1	1:C:271:TYR:CZ	2.69	0.44
1:E:269:LYS:NZ	1:E:352:GLU:OE2	2.50	0.44
1:A:320:GLU:OE2	1:A:322:ILE:HG22	2.17	0.44
1:K:270:LEU:O	1:K:274:ARG:HG3	2.17	0.44
2:B:43:GLN:HB2	2:B:49:LEU:HD23	2.00	0.44
1:K:236:VAL:HG21	1:K:319:MET:HE2	2.00	0.44
1:I:301:LYS:HE3	1:I:398:ARG:HE	1.82	0.44
2:L:102:THR:HG22	2:L:103:ASP:N	2.33	0.44
2:D:103:ASP:O	2:D:103:ASP:OD1	2.35	0.44
1:E:299:PHE:CZ	1:E:365:VAL:HG21	2.53	0.44
2:F:56:ASP:O	2:F:60:GLY:N	2.51	0.44
2:L:58:GLU:HB2	2:L:107:SER:OG	2.17	0.44
2:F:7:GLN:HB2	2:F:29:SER:HB2	2.00	0.43
1:G:221:ARG:NE	1:G:226:ARG:HD3	2.32	0.43
1:K:278:TYR:O	1:K:282:VAL:HG23	2.18	0.43
2:F:38:MET:H	2:F:102:THR:HG22	1.82	0.43
1:E:367:LYS:HD3	2:F:194:TYR:CE2	2.54	0.43
2:B:200:PRO:HD2	2:B:203:VAL:HG21	2.01	0.43
1:C:368:ARG:HG3	1:C:368:ARG:HH11	1.84	0.43
1:A:304:ARG:HG3	1:A:382:ALA:HA	2.01	0.43
1:A:370:LYS:HE2	2:B:113:ASP:OD2	2.17	0.43
1:C:370:LYS:O	2:D:104:PHE:CZ	2.72	0.43
1:C:429:VAL:HG12	1:C:431:PRO:HD2	2.00	0.43
1:K:232:THR:CG2	1:K:322:ILE:CD1	2.96	0.43
1:C:270:LEU:O	1:C:274:ARG:HG3	2.18	0.43
1:G:236:VAL:HG21	1:G:319:MET:HE3	2.01	0.43
2:J:102:THR:HG22	2:J:103:ASP:N	2.34	0.43
1:A:462:ASN:CB	1:E:374:ILE:HG23	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:HIS:HB2	2:H:112:PHE:CE2	2.54	0.43
1:K:269:LYS:NZ	1:K:352:GLU:OE2	2.51	0.43
2:L:184:LEU:HD12	2:L:184:LEU:H	1.83	0.43
1:A:364:SER:HB2	1:A:368:ARG:HH11	1.84	0.43
2:D:39:HIS:NE2	2:D:110:TYR:CE2	2.83	0.43
1:E:364:SER:O	1:E:368:ARG:CG	2.56	0.43
1:K:314:ILE:O	1:K:346:ARG:NE	2.42	0.43
2:B:58:GLU:HG2	2:B:107:SER:OG	2.18	0.42
1:C:369:LEU:HD12	1:C:371:GLY:O	2.19	0.42
2:D:67:LYS:O	2:D:68:PHE:HD1	2.02	0.42
2:L:57:ARG:NH2	2:L:76:GLU:OE2	2.51	0.42
2:D:237:ASP:OD2	2:D:240:LEU:N	2.46	0.42
1:E:250:LEU:O	1:E:253:LEU:HD13	2.20	0.42
1:A:364:SER:HB2	1:A:368:ARG:NH1	2.34	0.42
2:B:181:PHE:HE1	2:B:191:LEU:HD23	1.84	0.42
1:C:331:ASN:O	1:C:335:ILE:HG13	2.19	0.42
1:C:404:LEU:HB3	1:C:405:PRO:HD3	2.01	0.42
1:G:299:PHE:CZ	1:G:365:VAL:HG21	2.55	0.42
1:G:419:ILE:HG23	1:G:420:ASN:N	2.33	0.42
2:L:28:VAL:HG11	2:L:38:MET:HE3	2.00	0.42
2:B:28:VAL:HG13	2:B:38:MET:HE3	2.02	0.42
1:C:369:LEU:HD11	1:C:372:ASN:O	2.20	0.42
2:D:39:HIS:HA	2:D:54:GLY:HA2	2.02	0.42
1:E:430:PRO:HB2	1:E:431:PRO:HD3	2.02	0.42
2:F:33:LEU:O	2:F:33:LEU:HD23	2.20	0.42
1:K:430:PRO:HB2	1:K:431:PRO:HD3	2.01	0.42
2:B:6:VAL:HB	2:B:114:ILE:CD1	2.49	0.42
1:I:404:LEU:HB3	1:I:405:PRO:HD3	2.02	0.42
1:K:301:LYS:HG3	1:K:398:ARG:NH1	2.35	0.41
2:L:230:ASP:OD1	2:L:250:LYS:HG2	2.20	0.41
1:E:363:TYR:HD1	2:F:105:GLY:C	2.21	0.41
1:K:243:TYR:CE1	1:K:320:GLU:OE2	2.74	0.41
1:K:299:PHE:CZ	1:K:365:VAL:HG21	2.55	0.41
2:L:160:GLN:O	2:L:223:LEU:HB2	2.20	0.41
1:C:359:THR:CG2	2:D:107:SER:OG	2.68	0.41
1:E:363:TYR:CD1	2:F:105:GLY:O	2.52	0.41
2:H:33:LEU:HD23	2:H:33:LEU:O	2.21	0.41
2:J:39:HIS:HE2	2:J:110:TYR:HE1	1.68	0.41
1:A:320:GLU:CG	1:A:322:ILE:HG22	2.49	0.41
2:H:172:ASN:OD1	2:H:173:ILE:N	2.53	0.41
2:H:67:LYS:O	2:H:68:PHE:HD1	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:107:SER:O	2:J:108:TYR:HD1	2.04	0.41
1:K:268:ARG:HG3	1:K:269:LYS:N	2.36	0.41
1:E:404:LEU:HB3	1:E:405:PRO:HD3	2.02	0.41
1:C:364:SER:O	1:C:368:ARG:HG3	2.21	0.41
2:H:206:ARG:HH12	2:H:227:ASP:CG	2.23	0.41
1:I:370:LYS:HB2	1:I:370:LYS:HE3	1.87	0.41
2:J:228:GLU:OE2	2:J:252:THR:HG22	2.20	0.41
1:C:368:ARG:O	1:C:369:LEU:HB3	2.21	0.41
1:C:419:ILE:HG23	1:C:420:ASN:N	2.34	0.41
2:L:33:LEU:HD23	2:L:33:LEU:O	2.21	0.41
2:B:28:VAL:HG11	2:B:38:MET:HE1	2.02	0.41
1:K:450:TRP:CZ3	1:K:478:LEU:HD11	2.56	0.41
1:E:222:LYS:N	1:E:222:LYS:HD2	2.36	0.41
2:H:7:GLN:HB2	2:H:29:SER:HB2	2.02	0.41
1:A:224:ARG:NH2	1:A:399:ASP:HA	2.36	0.41
1:A:319:MET:HE1	1:A:456:LYS:HG2	2.03	0.41
1:I:418:LYS:HE3	1:I:422:THR:HA	2.03	0.41
1:E:242:ARG:O	1:E:242:ARG:NH1	2.49	0.40
1:C:421:TYR:OH	1:K:368:ARG:HD3	2.20	0.40
2:F:38:MET:HG3	2:F:83:VAL:HG21	2.02	0.40
1:G:430:PRO:HB2	1:G:431:PRO:HD3	2.02	0.40
1:I:367:LYS:O	1:I:370:LYS:HG3	2.21	0.40
2:B:227:ASP:OD2	2:B:251:LEU:CD1	2.69	0.40
2:F:43:GLN:O	2:F:96:ALA:HB1	2.22	0.40
2:J:224:GLN:O	2:J:225:SER:HB2	2.22	0.40
2:B:172:ASN:OD1	2:B:173:ILE:N	2.54	0.40
2:B:229:ALA:HB3	2:B:231:TYR:HE1	1.87	0.40
1:G:236:VAL:HG21	1:G:319:MET:CE	2.52	0.40
2:H:47:LYS:H	2:H:47:LYS:HD2	1.87	0.40
2:B:8:LEU:HG	2:B:114:ILE:HG22	2.03	0.40
1:C:222:LYS:H	1:C:222:LYS:HD2	1.87	0.40
1:C:242:ARG:HG3	1:C:320:GLU:OE1	2.21	0.40
1:C:418:LYS:HE3	1:C:422:THR:HA	2.03	0.40
2:F:172:ASN:OD1	2:F:173:ILE:N	2.54	0.40
1:G:419:ILE:HD13	1:G:428:LYS:HD3	2.04	0.40
2:H:95:THR:HG23	2:H:122:THR:HA	2.03	0.40

There are no symmetry-related clashes.

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	280/315 (89%)	269 (96%)	11 (4%)	0	100	100
1	C	282/315 (90%)	268 (95%)	14 (5%)	0	100	100
1	E	281/315 (89%)	267 (95%)	14 (5%)	0	100	100
1	G	280/315 (89%)	267 (95%)	13 (5%)	0	100	100
1	I	283/315 (90%)	269 (95%)	14 (5%)	0	100	100
1	K	281/315 (89%)	267 (95%)	14 (5%)	0	100	100
2	B	223/251 (89%)	206 (92%)	17 (8%)	0	100	100
2	D	223/251 (89%)	205 (92%)	18 (8%)	0	100	100
2	F	225/251 (90%)	208 (92%)	17 (8%)	0	100	100
2	H	225/251 (90%)	210 (93%)	15 (7%)	0	100	100
2	J	224/251 (89%)	205 (92%)	19 (8%)	0	100	100
2	L	223/251 (89%)	205 (92%)	18 (8%)	0	100	100
All	All	3030/3396 (89%)	2846 (94%)	184 (6%)	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	261/291 (90%)	256 (98%)	5 (2%)	57	80
1	C	265/291 (91%)	261 (98%)	4 (2%)	65	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	262/291 (90%)	261 (100%)	1 (0%)	91	96
1	G	261/291 (90%)	257 (98%)	4 (2%)	65	84
1	I	264/291 (91%)	262 (99%)	2 (1%)	81	91
1	K	262/291 (90%)	260 (99%)	2 (1%)	81	91
2	B	188/199 (94%)	186 (99%)	2 (1%)	73	88
2	D	188/199 (94%)	188 (100%)	0	100	100
2	F	190/199 (96%)	190 (100%)	0	100	100
2	H	190/199 (96%)	188 (99%)	2 (1%)	73	88
2	J	189/199 (95%)	188 (100%)	1 (0%)	88	94
2	L	188/199 (94%)	187 (100%)	1 (0%)	88	94
All	All	2708/2940 (92%)	2684 (99%)	24 (1%)	78	90

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	ASP
1	A	267	PHE
1	A	368	ARG
1	A	370	LYS
1	A	416	ASP
2	B	113	ASP
2	B	230	ASP
1	C	259	THR
1	C	267	PHE
1	C	465	LYS
1	C	475	TYR
1	E	267	PHE
1	G	264	ASP
1	G	267	PHE
1	G	319	MET
1	G	468	THR
2	H	28	VAL
2	H	230	ASP
1	I	267	PHE
1	I	372	ASN
2	J	225	SER
1	K	264	ASP
1	K	267	PHE
2	L	198	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	39	HIS
2	L	196	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
3	SO4	E	601	-	4,4,4	1.24	0	6,6,6	0.45	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	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, 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	284/315 (90%)	0.06	4 (1%) 75 69	67, 84, 113, 123	0
1	C	288/315 (91%)	-0.02	6 (2%) 63 58	56, 77, 107, 134	0
1	E	285/315 (90%)	-0.07	1 (0%) 92 90	53, 71, 101, 126	0
1	G	284/315 (90%)	0.04	3 (1%) 80 75	63, 82, 108, 116	0
1	I	287/315 (91%)	-0.01	5 (1%) 70 64	56, 75, 108, 127	0
1	K	285/315 (90%)	-0.04	2 (0%) 87 83	49, 70, 103, 119	0
2	B	227/251 (90%)	0.22	7 (3%) 49 43	82, 109, 130, 138	0
2	D	227/251 (90%)	0.10	3 (1%) 77 71	64, 85, 102, 113	0
2	F	229/251 (91%)	0.26	8 (3%) 44 39	75, 99, 129, 155	0
2	H	229/251 (91%)	0.20	4 (1%) 70 64	79, 109, 131, 138	0
2	J	228/251 (90%)	0.14	1 (0%) 92 90	67, 92, 117, 137	0
2	L	227/251 (90%)	0.10	3 (1%) 77 71	71, 94, 127, 147	0
All	All	3080/3396 (90%)	0.07	47 (1%) 73 68	49, 86, 122, 155	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	255	ASN	4.7
2	B	228	GLU	4.6
1	C	270	LEU	3.7
1	C	268	ARG	3.7
2	D	107	SER	3.2
1	C	255	ASN	3.1
1	C	218	ASN	3.1
1	G	218	ASN	3.1
1	I	218	ASN	3.0
1	I	268	ARG	3.0
1	I	269	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	107	SER	2.8
2	B	90	LEU	2.8
1	A	269	LYS	2.7
1	I	256	ASN	2.7
2	F	152	PRO	2.6
2	D	18	PRO	2.6
1	A	270	LEU	2.6
2	D	20	ALA	2.5
1	K	270	LEU	2.5
2	F	67	LYS	2.5
2	B	152	PRO	2.5
2	L	228	GLU	2.4
2	F	66	GLN	2.4
2	L	107	SER	2.4
2	F	147	VAL	2.4
2	F	91	ARG	2.4
2	B	161	ARG	2.4
2	B	162	VAL	2.3
1	C	264	ASP	2.3
1	K	508	SER	2.3
1	E	267	PHE	2.3
2	B	107	SER	2.3
2	H	16	LYS	2.3
1	G	322	ILE	2.2
2	H	4	SER	2.2
2	L	121	VAL	2.2
1	C	269	LYS	2.2
2	F	124	SER	2.2
2	H	11	SER	2.2
2	J	221	SER	2.1
2	F	123	VAL	2.1
2	F	168	GLY	2.1
1	A	218	ASN	2.1
1	A	421	TYR	2.1
2	B	151	SER	2.0
1	G	324	TYR	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 [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
3	SO4	E	601	5/5	0.89	0.31	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.