



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:02 AM UTC

PDB ID : 6OAO / pdb_00006oao
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 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

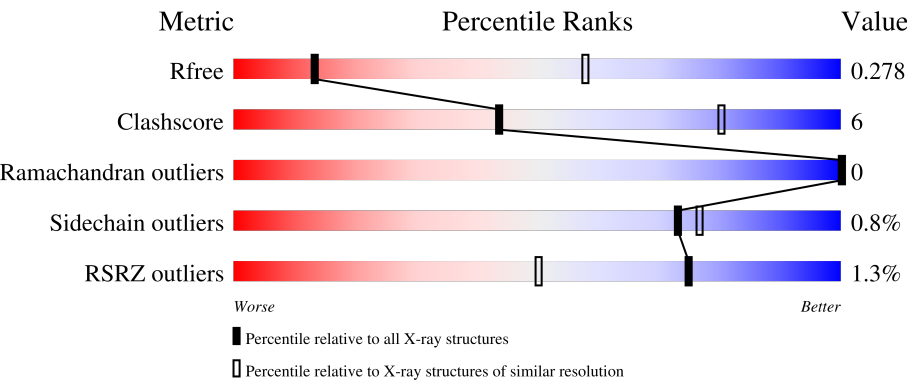
1 Overall quality at a glance i

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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	315	% 79%10%•10%
1	C	315	2% 78%13%9%
1	E	315	78%12%10%
1	G	315	% 80%10%10%
1	I	315	% 85%5%•9%

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Mol	Chain	Length	Quality of chain
1	K	315	% 77% 13% 10%
2	B	251	% 75% 14% 10%
2	D	251	% 77% 13% 10%
2	F	251	2% 80% 12% 9%
2	H	251	78% 13% 9%
2	J	251	2% 78% 12% 9%
2	L	251	2% 82% 8% 10%

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 (CCD ID: SO4) (formula: O₄S).



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

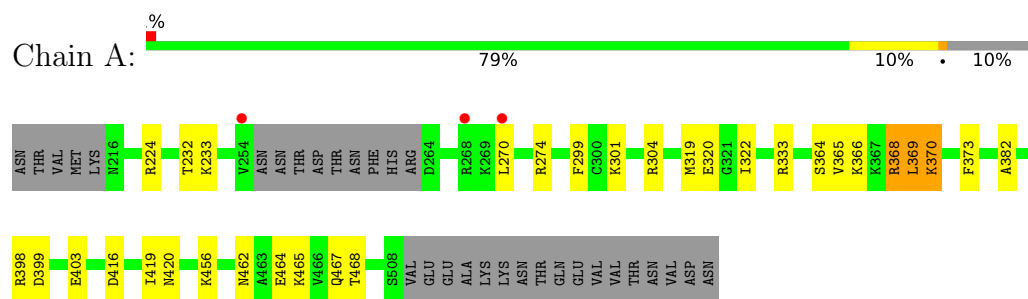
- Molecule 4 is water.

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		

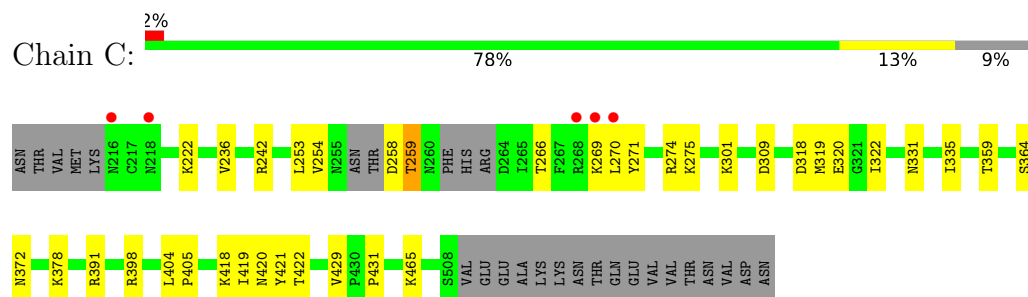
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

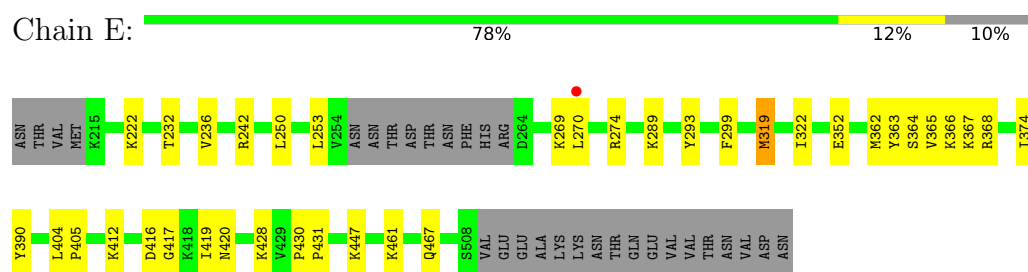
- Molecule 1: Duffy binding surface protein region II



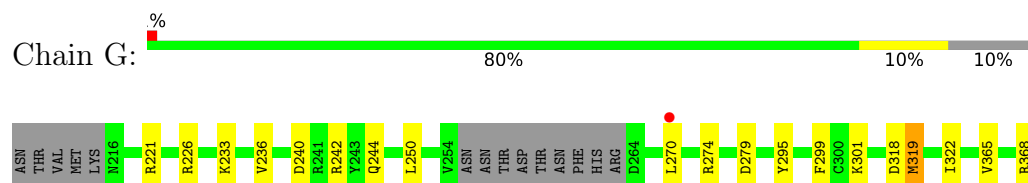
- Molecule 1: Duffy binding surface protein region II

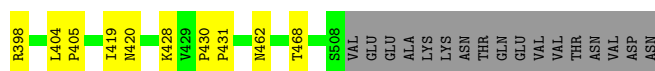


- Molecule 1: Duffy binding surface protein region II

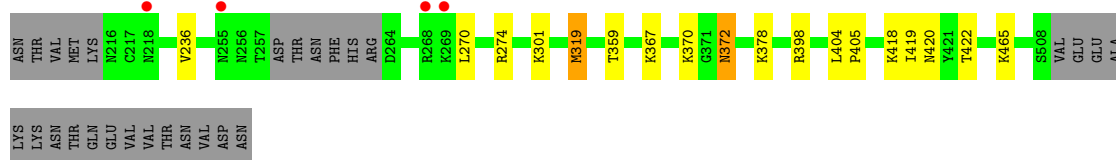
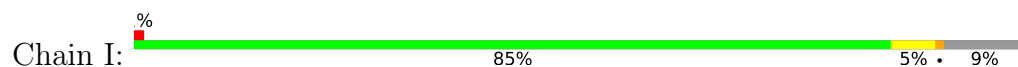


- Molecule 1: Duffy binding surface protein region II

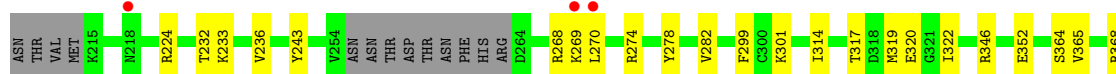
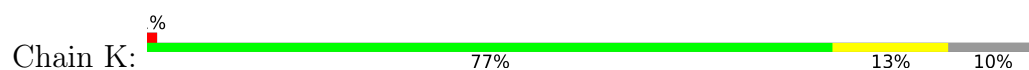




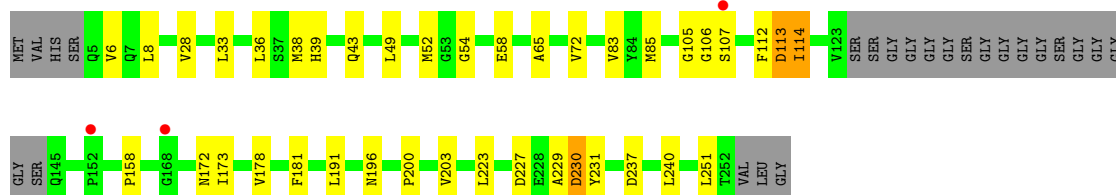
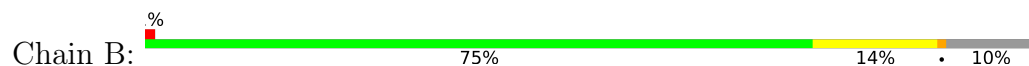
- Molecule 1: Duffy binding surface protein region II



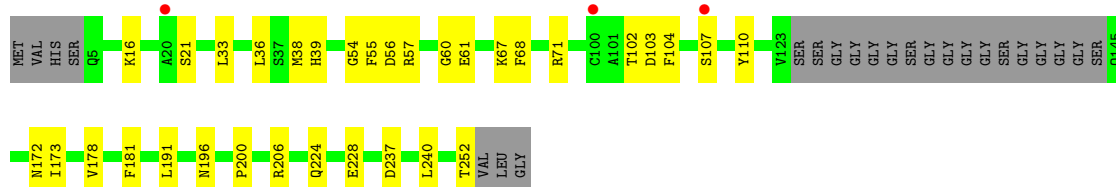
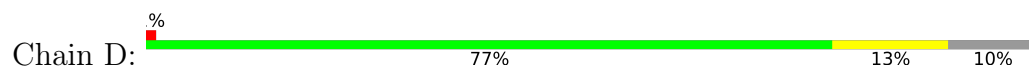
- Molecule 1: Duffy binding surface protein region II



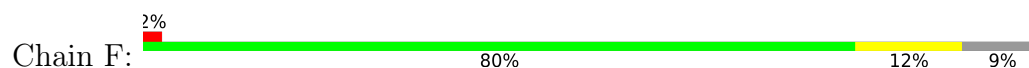
- Molecule 2: Antibody 092096 single chain variable fragment



- 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	130.66Å 89.56Å 193.71Å 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) 99.0 (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 3.52Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.237 , 0.279 0.242 , 0.278	Depositor DCC
R_{free} test set	2787 reflections (5.13%)	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 , 51.5	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	0.25	0/2420	0.42	0/3254
1	C	0.28	0/2450	0.44	0/3294
1	E	0.30	0/2429	0.45	0/3265
1	G	0.24	0/2420	0.40	0/3254
1	I	0.24	0/2443	0.41	0/3286
1	K	0.31	0/2429	0.46	0/3265
2	B	0.36	1/1749 (0.1%)	0.53	0/2371
2	D	0.36	0/1749	0.56	0/2371
2	F	0.51	3/1762 (0.2%)	0.59	2/2389 (0.1%)
2	H	0.31	1/1766 (0.1%)	0.47	0/2394
2	J	0.29	0/1755	0.45	0/2379
2	L	0.37	0/1749	0.51	0/2371
All	All	0.32	5/25121 (0.0%)	0.47	2/33893 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	109	PHE	C-N	8.00	1.45	1.33
2	F	69	GLN	C-N	-6.54	1.24	1.33
2	F	106	GLY	CA-C	-6.44	1.47	1.52
2	B	106	GLY	CA-C	-6.09	1.48	1.52
2	H	65	ALA	C-N	-5.98	1.26	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	109	PHE	CA-C-N	-6.61	110.51	122.54
2	F	109	PHE	C-N-CA	-6.61	110.51	122.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2374	0	2371	32	0
1	C	2405	0	2393	37	0
1	E	2383	0	2384	37	0
1	G	2374	0	2371	22	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	25	0
2	F	1725	0	1622	23	0
2	H	1728	0	1620	24	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	296	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 (296) 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:HE1	1:E:377:CYS:SG	1.97	1.04
1:E:364:SER:O	1:E:368:ARG:HG3	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:178:VAL:HB	2:L:196:ASN:ND2	1.88	0.89
1:E:363:TYR:HD1	2:F:105:GLY:O	1.59	0.83
2:B:28:VAL:CG1	2:B:38:MET:HE1	2.08	0.83
1:K:319:MET:HE3	1:K:456:LYS:HE2	1.66	0.77
2:J:102:THR:HG22	2:J:104:PHE:H	1.49	0.77
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
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: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
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
2:D:60:GLY:O	2:D:61:GLU:C	2.40	0.63
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:I:236:VAL:HG21	1:I:319:MET:HE3	1.79	0.62
1:E:236:VAL:HG21	1:E:319:MET:HE3	1.82	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
1:E:362:MET:HE3	1:E:377:CYS:HB2	1.84	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:CE	2.79	0.59
2:D:55:PHE:CE1	2:D:60:GLY:HA2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:362:MET:CE	1:E:377:CYS:HB2	2.34	0.57
2:B:230:ASP:OD1	2:B:230:ASP:N	2.36	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
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:HG22	1:K:317:THR:O	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:H:33:LEU:O	2:H:57:ARG:NH1	2.39	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
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
2:F:8:LEU:HD21	2:F:38:MET:HE1	1.89	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:HG3	1:K:368:ARG:HH11	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
1:E:447:LYS:NZ	3:E:601:SO4:O3	2.32	0.53
1:G:236:VAL:HG21	1:G:319:MET:HE3	1.90	0.53
1:A:319:MET:HE3	1:A:456:LYS:HE2	1.90	0.53
2:F:193:ILE:HD12	2:F:218:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:378:LYS:HG3	1:E:467:GLN:HB3	1.91	0.52
2:J:26:CYS:SG	2:J:38:MET:HE1	2.50	0.52
1:C:253:LEU:CD2	1:C:275:LYS:HG3	2.40	0.52
2:B:28:VAL:HG12	2:B:38:MET:HE1	1.90	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
2:L:58:GLU:HB2	2:L:107:SER:CB	2.40	0.51
1:G:368:ARG:HG3	1:G:368:ARG:HH11	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
1:E:362:MET:HE1	1:E:377:CYS:CB	2.41	0.50
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:E:362:MET:CE	1:E:377:CYS:CB	2.90	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
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:C:236:VAL:HG21	1:C:319:MET:HE3	1.94	0.49
1:A:270:LEU:O	1:A:274:ARG:HG3	2.12	0.49
1:C:242:ARG:HH21	1:C:318:ASP:CG	2.21	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: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
2:J:36:LEU:HB3	2:J:102:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:467:GLN:O	1:E:467:GLN:HG3	2.14	0.47
1:A:465:LYS:O	1:A:465:LYS:HG3	2.13	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:E:419:ILE:HD13	1:E:428:LYS:HD3	1.96	0.47
1:G:221:ARG:CZ	1:G:226:ARG:HH11	2.27	0.47
1:I:372:ASN:O	1:I:372:ASN:ND2	2.46	0.47
1:I:378:LYS:NZ	1:K:461:LYS:O	2.40	0.47
2:J:33:LEU:HD23	2:J:33:LEU:O	2.15	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
2:H:42:ARG:HH21	2:H:68:PHE:HZ	1.63	0.47
2:B:36:LEU:N	2:B:36:LEU:HD12	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:E:363:TYR:HD1	2:F:105:GLY:C	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:206:ARG:HH12	2:H:227:ASP:CG	2.23	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: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
2:D:102:THR:HG22	2:D:103:ASP:N	2.30	0.45
2:H:43:GLN:HB2	2:H:49:LEU:HD23	1.99	0.45
2:H:158:PRO:HA	2:H:223:LEU:O	2.17	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:G:462:ASN:HB3	1:K:374:ILE:HG23	1.98	0.45
1:I:270:LEU:O	1:I:274:ARG:HG3	2.17	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
1:A:224:ARG:HD3	1:A:403:GLU:CG	2.48	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
2:L:8:LEU:HD21	2:L:38:MET:HE1	2.00	0.44
2:L:196:ASN:CG	2:L:211:LYS:HD3	2.43	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:OD1	2:D:103:ASP:O	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:H:36:LEU:HD22	2:H:38:MET:HE2	2.00	0.44
2:J:224:GLN:C	2:J:226:GLU:H	2.24	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
1:E:367:LYS:HD3	2:F:194:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:38:MET:H	2:F:102:THR:HG22	1.82	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
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
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:H	2:L:184:LEU:HD12	1.83	0.43
1:A:364:SER:HB2	1:A:368:ARG:HH11	1.84	0.43
1:A:467:GLN:C	1:A:468:THR:HG22	2.44	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:E:362:MET:CE	1:E:377:CYS:SG	2.87	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:270:LEU:HD23	1:C:270:LEU:C	2.45	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
2:H:103:ASP:C	2:H:105:GLY:H	2.28	0.42
2:B:72:VAL:HG23	2:B:85:MET:HE2	2.00	0.42
1:G:419:ILE:HG23	1:G:420:ASN:N	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O	2:H:33:LEU:HD23	2.21	0.41
1:K:236:VAL:HG21	1:K:319:MET:HE2	2.03	0.41
1:A:320:GLU:CG	1:A:322:ILE:HG22	2.49	0.41
2:B:28:VAL:HG11	2:B:38:MET:HE1	1.95	0.41
1:E:363:TYR:CD1	2:F:105:GLY:C	2.99	0.41
2:H:67:LYS:O	2:H:68:PHE:HD1	2.02	0.41
2:H:172:ASN:OD1	2:H:173:ILE:N	2.53	0.41
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
1:G:242:ARG:HH21	1:G:318:ASP:CG	2.29	0.41
1:I:370:LYS:HE3	1:I:370:LYS:HB2	1.87	0.41
2:J:228:GLU:OE2	2:J:252:THR:HG22	2.20	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
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:K:450:TRP:CZ3	1:K:478:LEU:HD11	2.56	0.41
1:A:224:ARG:NH2	1:A:399:ASP:HA	2.36	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:HD2	2:H:47:LYS:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:LEU:HG	2:B:114:ILE:HG22	2.03	0.40
1:C:222:LYS:HD2	1:C:222:LYS:H	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 [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	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%)	257 (98%)	4 (2%)	57	71
1	C	265/291 (91%)	262 (99%)	3 (1%)	65	74
1	E	262/291 (90%)	261 (100%)	1 (0%)	84	81
1	G	261/291 (90%)	259 (99%)	2 (1%)	73	77
1	I	264/291 (91%)	262 (99%)	2 (1%)	73	77
1	K	262/291 (90%)	262 (100%)	0	100	100
2	B	188/199 (94%)	185 (98%)	3 (2%)	55	70
2	D	188/199 (94%)	187 (100%)	1 (0%)	81	80
2	F	190/199 (96%)	190 (100%)	0	100	100
2	H	190/199 (96%)	188 (99%)	2 (1%)	65	74
2	J	189/199 (95%)	186 (98%)	3 (2%)	55	70
2	L	188/199 (94%)	187 (100%)	1 (0%)	81	80
All	All	2708/2940 (92%)	2686 (99%)	22 (1%)	73	77

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	ARG
1	A	369	LEU
1	A	370	LYS
1	A	416	ASP
2	B	113	ASP
2	B	114	ILE
2	B	230	ASP
1	C	259	THR
1	C	322	ILE
1	C	465	LYS
2	D	71	ARG
1	E	319	MET
1	G	319	MET
1	G	468	THR

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Mol	Chain	Res	Type
2	H	28	VAL
2	H	230	ASP
1	I	319	MET
1	I	372	ASN
2	J	28	VAL
2	J	223	LEU
2	J	225	SER
2	L	198	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	330	ASN
1	A	348	GLN
1	A	467	GLN
2	B	176	ASN
1	C	218	ASN
1	C	344	GLN
1	C	495	ASN
2	D	5	GLN
2	D	241	ASN
1	E	343	GLN
1	G	218	ASN
1	G	330	ASN
1	G	344	GLN
1	G	486	ASN
2	H	198	GLN
1	I	218	ASN
1	I	330	ASN
1	I	344	GLN
1	I	348	GLN
1	I	495	ASN
1	K	291	ASN
1	K	344	GLN
1	K	348	GLN
1	K	486	ASN
2	L	43	GLN
2	L	183	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 oligosaccharides 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	1.26	0	6,6,6	0.44	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%)	0.15	3 (1%) 78 54	67, 84, 113, 122	0
1	C	288/315 (91%)	0.04	6 (2%) 63 38	56, 77, 107, 134	0
1	E	285/315 (90%)	0.06	1 (0%) 88 72	53, 71, 101, 126	0
1	G	284/315 (90%)	0.05	2 (0%) 84 63	63, 82, 108, 116	0
1	I	287/315 (91%)	0.05	4 (1%) 73 48	56, 75, 108, 127	0
1	K	285/315 (90%)	0.06	4 (1%) 73 48	49, 70, 103, 119	0
2	B	227/251 (90%)	0.33	3 (1%) 75 50	82, 109, 130, 138	0
2	D	227/251 (90%)	0.24	3 (1%) 75 50	64, 85, 102, 113	0
2	F	229/251 (91%)	0.35	5 (2%) 62 37	75, 99, 129, 155	0
2	H	229/251 (91%)	0.26	1 (0%) 88 72	79, 109, 131, 138	0
2	J	228/251 (90%)	0.29	4 (1%) 67 42	67, 92, 117, 137	0
2	L	227/251 (90%)	0.24	5 (2%) 62 37	71, 94, 127, 147	0
All	All	3080/3396 (90%)	0.17	41 (1%) 75 50	49, 86, 122, 155	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	107	SER	5.4
2	H	107	SER	4.6
2	L	107	SER	4.2
2	F	107	SER	3.7
1	C	268	ARG	3.4
1	C	270	LEU	3.3
2	F	152	PRO	3.2
2	D	107	SER	3.0
1	C	369	LEU	2.8
1	G	270	LEU	2.8
1	C	218	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	J	38	MET	2.7
2	F	147	VAL	2.6
2	L	252	THR	2.5
1	K	270	LEU	2.5
1	I	255	ASN	2.4
1	I	268	ARG	2.4
2	J	62	SER	2.3
2	B	168	GLY	2.3
1	C	269	LYS	2.3
1	K	269	LYS	2.3
2	D	20	ALA	2.3
2	L	228	GLU	2.3
2	B	152	PRO	2.3
2	F	169	SER	2.3
1	A	270	LEU	2.3
2	F	17	LYS	2.3
1	A	268	ARG	2.3
1	G	374	ILE	2.2
1	C	216	ASN	2.2
2	J	222	GLY	2.2
1	K	218	ASN	2.2
2	J	196	ASN	2.2
1	E	270	LEU	2.1
1	K	504	LEU	2.1
1	A	254	VAL	2.1
1	I	269	LYS	2.1
2	L	235	ALA	2.1
2	L	201	SER	2.0
2	D	100	CYS	2.0
1	I	218	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	E	601	5/5	0.84	0.33	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.