Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 03:35 PM JST

PDB ID	:	6JJJ
Title	:	Trimeric structure of Kupffer cell C-type lectin receptor Clec4f
Authors	:	Wen, Y.; Ouyang, Z.; Felix, J.
Deposited on	:	2019-02-26
Resolution	:	2.79 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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:

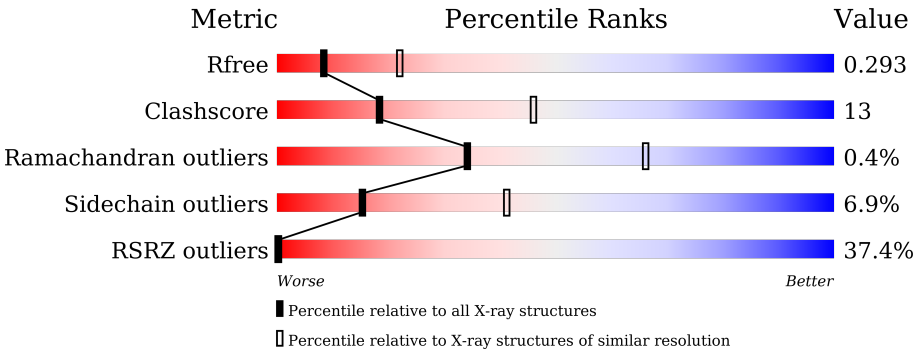
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	160	32% 69% 22% • 6%
1	B	160	33% 67% 24% • 6%
1	C	160	36% 73% 19% • 6%
1	D	160	36% 74% 19% • 6%
1	E	160	38% 65% 27% • 6%
1	F	160	38% 71% 19% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14037 atoms, of which 6649 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 C-type lectin domain family 4 member F.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	151	Total	C	H	N	O	S	0	0	0
			2304	763	1090	216	230	5			
1	B	151	Total	C	H	N	O	S	0	0	0
			2341	770	1112	223	231	5			
1	C	151	Total	C	H	N	O	S	0	0	0
			2341	770	1112	223	231	5			
1	D	151	Total	C	H	N	O	S	0	0	0
			2343	771	1111	224	232	5			
1	E	151	Total	C	H	N	O	S	0	0	0
			2345	773	1112	224	231	5			
1	F	151	Total	C	H	N	O	S	0	0	0
			2345	773	1112	224	231	5			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		
2	D	2	Total	Ca	0	0
			2	2		
2	E	2	Total	Ca	0	0
			2	2		
2	F	2	Total	Ca	0	0
			2	2		

- Molecule 3 is water.

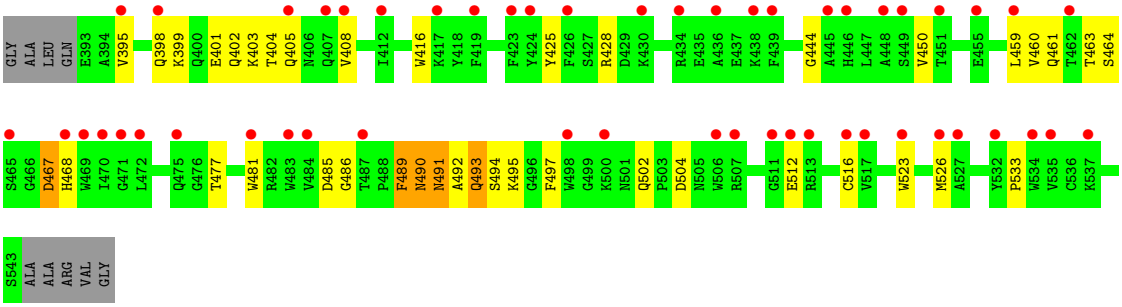
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0
3	E	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

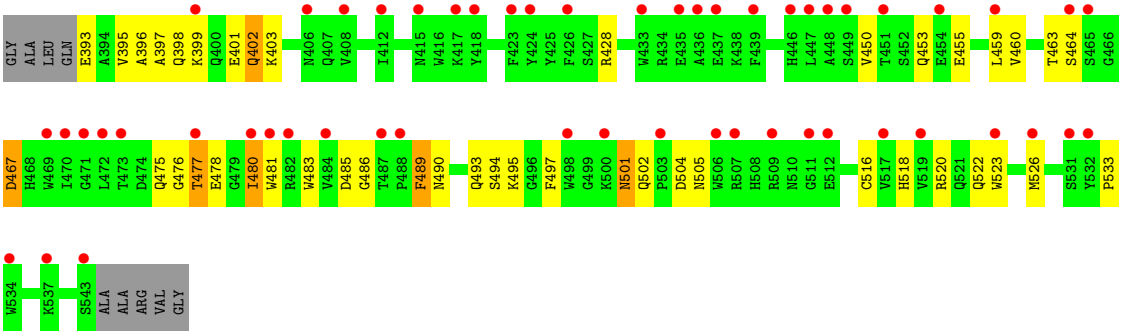
• Molecule 1: C-type lectin domain family 4 member F

Chain A:



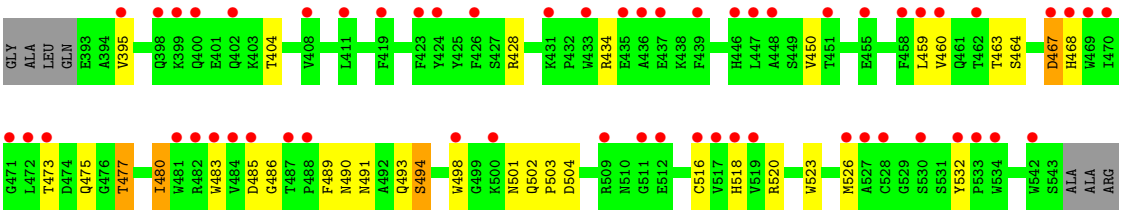
• Molecule 1: C-type lectin domain family 4 member F

Chain B:

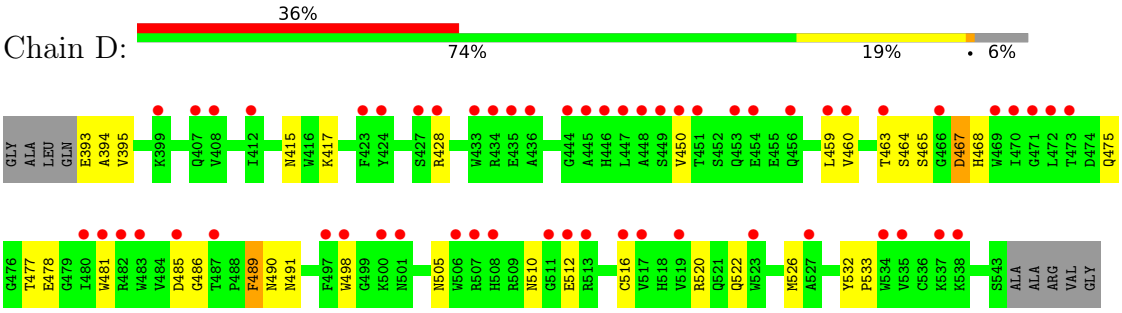


• Molecule 1: C-type lectin domain family 4 member F

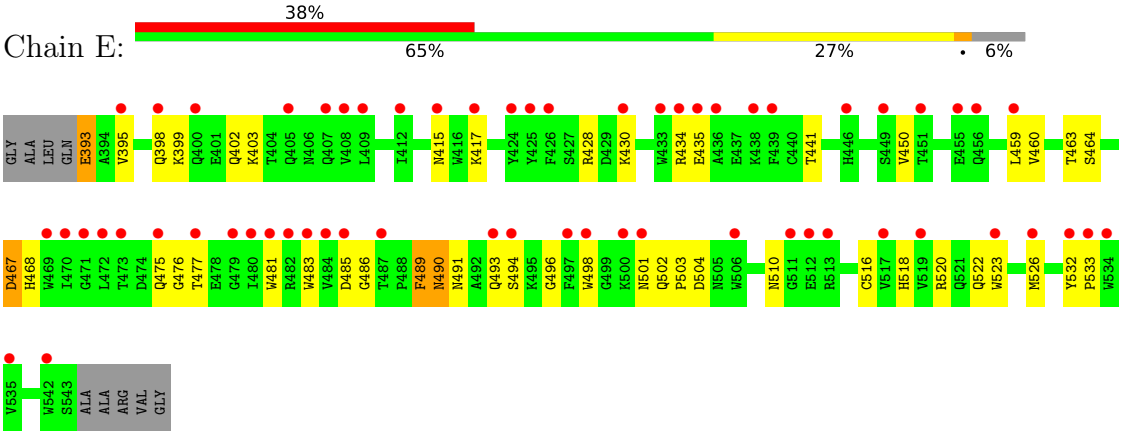
Chain C:



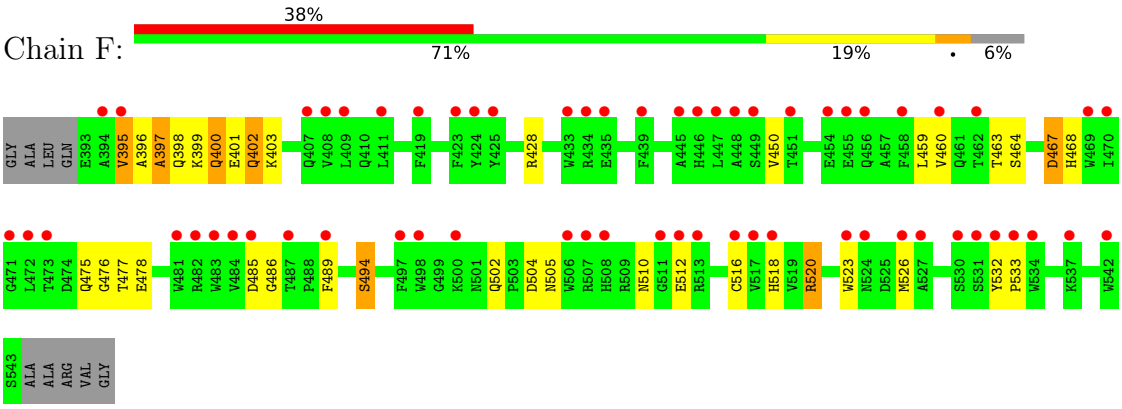
• Molecule 1: C-type lectin domain family 4 member F



• Molecule 1: C-type lectin domain family 4 member F



• Molecule 1: C-type lectin domain family 4 member F



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	75.15Å 75.19Å 61.20Å 90.01° 90.04° 120.06°	Depositor
Resolution (Å)	32.56 – 2.79 44.60 – 2.79	Depositor EDS
% Data completeness (in resolution range)	93.8 (32.56-2.79) 94.1 (44.60-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.250 , 0.292 0.250 , 0.293	Depositor DCC
R_{free} test set	2621 reflections (9.64%)	wwPDB-VP
Wilson B-factor (Å^2)	95.9	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 124.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.021 for -k,h+k,l 0.021 for h+k,-h,l 0.460 for -h-k,h,l 0.460 for k,-h-k,l 0.024 for -h,-k,l 0.467 for k,h,-l 0.468 for h,-h-k,-l 0.022 for h+k,-k,-l 0.468 for -h-k,k,-l 0.020 for -k,-h,-l 0.022 for -h,h+k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14037	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.38	0/1252	0.50	0/1701
1	B	0.39	0/1267	0.50	0/1719
1	C	0.28	0/1267	0.45	0/1719
1	D	0.27	0/1270	0.44	0/1723
1	E	0.27	0/1271	0.46	0/1723
1	F	0.40	0/1271	0.50	0/1723
All	All	0.33	0/7598	0.47	0/10308

There are no bond length outliers.

There are no bond angle outliers.

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	1214	1090	1087	44	0
1	B	1229	1112	1113	45	0
1	C	1229	1112	1113	31	0
1	D	1232	1111	1117	19	0
1	E	1233	1112	1124	34	0
1	F	1233	1112	1124	33	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	7388	6649	6678	187	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 13.

All (187) 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:A:491:ASN:N	1:A:494:SER:OG	1.89	1.06
1:B:402:GLN:NE2	1:F:402:GLN:OE1	1.92	1.01
1:F:397:ALA:O	1:F:400:GLN:N	1.95	0.98
1:F:396:ALA:O	1:F:398:GLN:N	1.99	0.94
1:C:490:ASN:O	1:C:493:GLN:N	2.04	0.91
1:E:496:GLY:O	1:E:522:GLN:NE2	2.07	0.88
1:F:397:ALA:O	1:F:400:GLN:CB	2.23	0.87
1:B:397:ALA:O	1:B:398:GLN:C	2.14	0.83
1:B:460:VAL:O	1:B:464:SER:N	2.13	0.82
1:A:398:GLN:HB3	1:B:398:GLN:NE2	1.96	0.81
1:A:491:ASN:N	1:A:492:ALA:HB3	1.98	0.79
1:B:397:ALA:O	1:B:398:GLN:O	2.00	0.79
1:A:398:GLN:HB3	1:B:398:GLN:HE21	1.48	0.79
1:A:459:LEU:O	1:A:463:THR:HG22	1.85	0.76
1:A:398:GLN:HE22	1:F:399:LYS:HG3	1.51	0.75
1:E:498:TRP:O	1:E:522:GLN:NE2	2.20	0.75
1:B:459:LEU:O	1:B:463:THR:HG22	1.86	0.75
1:F:397:ALA:O	1:F:400:GLN:CA	2.34	0.74
1:E:393:GLU:N	1:E:393:GLU:OE2	2.21	0.74
1:A:492:ALA:O	1:A:494:SER:N	2.20	0.74
1:A:405:GLN:O	1:A:408:VAL:HG22	1.91	0.70
1:A:398:GLN:CB	1:B:398:GLN:NE2	2.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:OG1	1:C:468:HIS:ND1	2.20	0.69
1:F:467:ASP:OD1	1:F:467:ASP:N	2.24	0.69
1:E:460:VAL:O	1:E:464:SER:N	2.26	0.68
1:E:467:ASP:OD1	1:E:467:ASP:N	2.27	0.68
1:A:460:VAL:O	1:A:464:SER:N	2.26	0.67
1:E:490:ASN:HD21	1:E:493:GLN:CB	2.06	0.67
1:C:467:ASP:N	1:C:467:ASP:OD1	2.27	0.67
1:B:467:ASP:OD1	1:B:467:ASP:N	2.27	0.66
1:B:501:ASN:O	1:B:501:ASN:ND2	2.28	0.66
1:A:398:GLN:C	1:B:398:GLN:HE22	2.00	0.65
1:D:460:VAL:O	1:D:464:SER:N	2.30	0.65
1:B:478:GLU:OE2	1:B:505:ASN:ND2	2.31	0.64
1:D:510:ASN:O	1:D:512:GLU:N	2.30	0.64
1:E:399:LYS:HG2	1:E:403:LYS:HE3	1.77	0.64
1:A:481:TRP:HB2	1:A:489:PHE:HZ	1.63	0.64
1:F:397:ALA:O	1:F:400:GLN:HB2	1.97	0.64
1:F:510:ASN:O	1:F:512:GLU:N	2.30	0.63
1:C:516:CYS:O	1:C:526:MET:N	2.29	0.63
1:F:478:GLU:OE2	1:F:505:ASN:ND2	2.31	0.63
1:F:516:CYS:O	1:F:526:MET:N	2.32	0.63
1:D:467:ASP:N	1:D:467:ASP:OD1	2.30	0.63
1:D:516:CYS:O	1:D:526:MET:N	2.32	0.63
1:A:404:THR:O	1:A:405:GLN:C	2.38	0.62
1:E:516:CYS:O	1:E:526:MET:N	2.32	0.62
1:B:475:GLN:HE22	1:C:404:THR:HG21	1.65	0.61
1:C:473:THR:OG1	1:C:475:GLN:HG3	2.01	0.61
1:F:397:ALA:O	1:F:401:GLU:N	2.34	0.61
1:D:393:GLU:HG3	1:D:394:ALA:H	1.67	0.60
1:E:501:ASN:ND2	1:E:501:ASN:O	2.34	0.60
1:E:510:ASN:O	1:E:510:ASN:ND2	2.35	0.60
1:A:490:ASN:C	1:A:492:ALA:HB3	2.22	0.59
1:B:485:ASP:OD1	1:B:486:GLY:N	2.35	0.59
1:C:460:VAL:O	1:C:464:SER:N	2.36	0.59
1:E:502:GLN:OE1	1:E:504:ASP:N	2.34	0.59
1:D:478:GLU:OE2	1:D:505:ASN:ND2	2.34	0.59
1:A:516:CYS:O	1:A:526:MET:N	2.36	0.58
1:A:491:ASN:HA	1:A:493:GLN:N	2.18	0.58
1:C:395:VAL:HG23	1:C:395:VAL:O	2.03	0.58
1:B:395:VAL:O	1:B:395:VAL:HG23	2.02	0.58
1:F:460:VAL:O	1:F:464:SER:N	2.36	0.58
1:F:397:ALA:C	1:F:400:GLN:H	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:CYS:O	1:B:526:MET:N	2.36	0.58
1:A:481:TRP:HB2	1:A:489:PHE:CZ	2.39	0.57
1:B:403:LYS:HZ3	1:C:434:ARG:CZ	2.16	0.57
1:A:395:VAL:O	1:A:395:VAL:HG23	2.04	0.57
1:F:400:GLN:O	1:F:403:LYS:HB2	2.04	0.57
1:A:485:ASP:OD1	1:A:486:GLY:N	2.38	0.57
1:B:481:TRP:HB2	1:B:489:PHE:CZ	2.40	0.56
1:A:401:GLU:O	1:A:402:GLN:C	2.42	0.56
1:F:485:ASP:OD1	1:F:486:GLY:N	2.38	0.56
1:B:502:GLN:OE1	1:B:504:ASP:N	2.39	0.56
1:B:489:PHE:CG	1:B:490:ASN:N	2.72	0.55
1:A:490:ASN:N	1:A:492:ALA:HB3	2.21	0.55
1:C:485:ASP:OD1	1:C:486:GLY:N	2.40	0.55
1:F:502:GLN:OE1	1:F:504:ASP:N	2.40	0.55
1:B:475:GLN:HE22	1:C:404:THR:CG2	2.20	0.55
1:E:485:ASP:OD1	1:E:486:GLY:N	2.41	0.54
1:F:463:THR:HG1	1:F:468:HIS:CG	2.26	0.54
1:B:450:VAL:O	1:B:450:VAL:HG23	2.08	0.54
1:C:450:VAL:HG21	1:C:523:TRP:HZ2	1.72	0.54
1:B:398:GLN:O	1:B:399:LYS:C	2.46	0.53
1:A:489:PHE:CG	1:A:490:ASN:N	2.76	0.53
1:C:501:ASN:O	1:C:501:ASN:ND2	2.41	0.53
1:D:485:ASP:OD1	1:D:486:GLY:N	2.41	0.53
1:E:459:LEU:O	1:E:463:THR:HG22	2.09	0.53
1:C:502:GLN:OE1	1:C:504:ASP:N	2.42	0.53
1:A:398:GLN:NE2	1:F:399:LYS:HG3	2.23	0.52
1:C:450:VAL:HG21	1:C:523:TRP:CZ2	2.43	0.52
1:A:502:GLN:OE1	1:A:504:ASP:N	2.41	0.52
1:B:403:LYS:HZ3	1:C:434:ARG:NH1	2.06	0.52
1:B:403:LYS:NZ	1:C:434:ARG:CZ	2.72	0.52
1:D:415:ASN:OD1	1:D:417:LYS:HE2	2.10	0.51
1:F:400:GLN:O	1:F:403:LYS:N	2.41	0.51
1:B:497:PHE:O	1:B:522:GLN:HB3	2.10	0.51
1:B:450:VAL:HG21	1:B:523:TRP:CZ2	2.46	0.51
1:B:450:VAL:HG21	1:B:523:TRP:HZ2	1.76	0.51
1:F:398:GLN:O	1:F:402:GLN:N	2.29	0.50
1:B:497:PHE:O	1:B:523:TRP:N	2.40	0.50
1:C:459:LEU:O	1:C:463:THR:HG22	2.11	0.50
1:B:403:LYS:HZ1	1:C:434:ARG:NH2	2.09	0.50
1:A:491:ASN:CA	1:A:492:ALA:C	2.80	0.49
1:B:398:GLN:O	1:B:401:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:TRP:O	1:D:522:GLN:OE1	2.30	0.49
1:F:450:VAL:O	1:F:450:VAL:HG23	2.12	0.49
1:B:483:TRP:NE1	1:B:489:PHE:HB3	2.27	0.49
1:D:450:VAL:HG23	1:D:450:VAL:O	2.11	0.49
1:A:450:VAL:HG23	1:A:450:VAL:O	2.12	0.49
1:B:477:THR:OG1	1:B:480:ILE:HD12	2.12	0.49
1:A:401:GLU:O	1:A:403:LYS:N	2.45	0.49
1:B:450:VAL:HG22	1:B:483:TRP:CZ2	2.48	0.49
1:E:450:VAL:HG23	1:E:450:VAL:O	2.11	0.49
1:C:477:THR:OG1	1:C:480:ILE:HD12	2.12	0.49
1:C:490:ASN:O	1:C:493:GLN:CA	2.60	0.49
1:D:459:LEU:O	1:D:463:THR:HG22	2.13	0.48
1:A:468:HIS:CE1	1:A:533:PRO:HB2	2.48	0.48
1:D:395:VAL:O	1:D:395:VAL:HG13	2.12	0.48
1:B:396:ALA:O	1:B:399:LYS:N	2.46	0.48
1:C:450:VAL:O	1:C:450:VAL:HG23	2.13	0.48
1:A:398:GLN:C	1:B:398:GLN:NE2	2.66	0.48
1:E:395:VAL:O	1:E:395:VAL:HG13	2.14	0.48
1:C:490:ASN:HB3	1:C:493:GLN:CB	2.44	0.47
1:F:399:LYS:O	1:F:403:LYS:HG3	2.14	0.47
1:A:495:LYS:C	1:A:497:PHE:H	2.19	0.46
1:E:399:LYS:O	1:E:403:LYS:HG3	2.15	0.46
1:E:450:VAL:HG21	1:E:523:TRP:CZ2	2.51	0.46
1:A:467:ASP:N	1:A:467:ASP:OD1	2.49	0.46
1:A:491:ASN:HA	1:A:492:ALA:C	2.36	0.46
1:B:481:TRP:O	1:B:489:PHE:CE1	2.69	0.46
1:B:475:GLN:NE2	1:C:404:THR:HG21	2.29	0.45
1:A:444:GLY:CA	1:E:441:THR:HB	2.47	0.45
1:D:467:ASP:HB2	1:D:532:TYR:HD1	1.83	0.44
1:F:459:LEU:O	1:F:463:THR:HG22	2.16	0.44
1:A:450:VAL:HG21	1:A:523:TRP:HZ2	1.82	0.44
1:B:475:GLN:O	1:B:476:GLY:C	2.55	0.44
1:F:450:VAL:HG21	1:F:523:TRP:CZ2	2.53	0.44
1:E:491:ASN:HA	1:E:494:SER:OG	2.17	0.44
1:A:490:ASN:N	1:A:492:ALA:CB	2.81	0.43
1:E:475:GLN:O	1:E:476:GLY:C	2.57	0.43
1:D:467:ASP:O	1:D:533:PRO:HG2	2.19	0.43
1:F:397:ALA:HA	1:F:400:GLN:HB2	1.99	0.43
1:E:450:VAL:HG21	1:E:523:TRP:HZ2	1.83	0.43
1:E:502:GLN:HG3	1:E:503:PRO:HA	2.01	0.43
1:E:398:GLN:O	1:E:402:GLN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:467:ASP:HB2	1:F:532:TYR:CD1	2.54	0.43
1:F:494:SER:H	1:F:494:SER:HG	1.59	0.43
1:D:490:ASN:OD1	1:D:491:ASN:N	2.52	0.42
1:B:467:ASP:O	1:B:533:PRO:HG2	2.19	0.42
1:C:450:VAL:HG22	1:C:483:TRP:CZ2	2.54	0.42
1:E:467:ASP:O	1:E:533:PRO:HG2	2.19	0.42
1:E:459:LEU:O	1:E:463:THR:N	2.51	0.42
1:F:475:GLN:O	1:F:476:GLY:C	2.58	0.42
1:A:450:VAL:HG21	1:A:523:TRP:CZ2	2.55	0.42
1:A:416:TRP:CD2	1:A:425:TYR:HB2	2.55	0.42
1:A:444:GLY:HA3	1:E:441:THR:HB	2.00	0.42
1:B:450:VAL:HG22	1:B:483:TRP:CH2	2.54	0.42
1:E:434:ARG:CG	1:E:435:GLU:N	2.83	0.42
1:A:399:LYS:N	1:B:398:GLN:HE22	2.17	0.42
1:C:490:ASN:O	1:C:491:ASN:C	2.57	0.42
1:E:467:ASP:HB2	1:E:532:TYR:HD1	1.84	0.41
1:F:395:VAL:O	1:F:395:VAL:CG1	2.68	0.41
1:A:489:PHE:O	1:A:490:ASN:CB	2.68	0.41
1:B:489:PHE:O	1:B:490:ASN:CB	2.68	0.41
1:F:463:THR:HG1	1:F:468:HIS:CE1	2.37	0.41
1:C:467:ASP:HB2	1:C:532:TYR:CD1	2.55	0.41
1:D:463:THR:OG1	1:D:468:HIS:ND1	2.47	0.41
1:A:404:THR:CG2	1:E:475:GLN:HE22	2.33	0.41
1:C:491:ASN:O	1:C:493:GLN:O	2.38	0.41
1:F:467:ASP:O	1:F:533:PRO:HG2	2.19	0.41
1:C:494:SER:O	1:C:498:TRP:CD1	2.74	0.41
1:D:464:SER:O	1:D:465:SER:HB2	2.20	0.41
1:A:459:LEU:C	1:A:463:THR:HG22	2.40	0.41
1:E:450:VAL:HG22	1:E:483:TRP:CZ2	2.56	0.41
1:C:502:GLN:HG3	1:C:503:PRO:HA	2.03	0.41
1:E:415:ASN:OD1	1:E:417:LYS:HE2	2.21	0.41
1:E:491:ASN:O	1:E:494:SER:OG	2.33	0.41
1:A:490:ASN:O	1:A:491:ASN:CB	2.70	0.41
1:B:455:GLU:O	1:B:459:LEU:HD23	2.21	0.41
1:E:489:PHE:CD1	1:E:489:PHE:O	2.75	0.40
1:D:463:THR:HG1	1:D:468:HIS:CE1	2.38	0.40
1:D:481:TRP:HB2	1:D:489:PHE:CZ	2.56	0.40
1:C:463:THR:HG1	1:C:468:HIS:CE1	2.23	0.40
1:F:467:ASP:CG	1:F:520:ARG:HD2	2.42	0.40
1:A:491:ASN:HA	1:A:493:GLN:C	2.42	0.40
1:B:493:GLN:C	1:B:495:LYS:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:481:TRP:HB2	1:E:489:PHE:CE2	2.57	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	149/160 (93%)	131 (88%)	15 (10%)	3 (2%)	7 24
1	B	149/160 (93%)	135 (91%)	14 (9%)	0	100 100
1	C	149/160 (93%)	138 (93%)	11 (7%)	0	100 100
1	D	149/160 (93%)	138 (93%)	11 (7%)	0	100 100
1	E	149/160 (93%)	138 (93%)	11 (7%)	0	100 100
1	F	149/160 (93%)	138 (93%)	10 (7%)	1 (1%)	22 53
All	All	894/960 (93%)	818 (92%)	72 (8%)	4 (0%)	34 66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	ASN
1	A	493	GLN
1	F	397	ALA
1	A	491	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	123/133 (92%)	117 (95%)	6 (5%)	25 57
1	B	126/133 (95%)	114 (90%)	12 (10%)	8 25
1	C	126/133 (95%)	118 (94%)	8 (6%)	18 46
1	D	127/133 (96%)	121 (95%)	6 (5%)	26 59
1	E	127/133 (96%)	117 (92%)	10 (8%)	12 34
1	F	127/133 (96%)	117 (92%)	10 (8%)	12 34
All	All	756/798 (95%)	704 (93%)	52 (7%)	15 41

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	428	ARG
1	A	461	GLN
1	A	467	ASP
1	A	477	THR
1	A	489	PHE
1	A	512	GLU
1	B	393	GLU
1	B	402	GLN
1	B	428	ARG
1	B	453	GLN
1	B	467	ASP
1	B	477	THR
1	B	480	ILE
1	B	489	PHE
1	B	494	SER
1	B	501	ASN
1	B	518	HIS
1	B	520	ARG
1	C	428	ARG
1	C	467	ASP
1	C	477	THR
1	C	480	ILE
1	C	489	PHE
1	C	494	SER
1	C	518	HIS
1	C	520	ARG
1	D	428	ARG
1	D	467	ASP

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Mol	Chain	Res	Type
1	D	475	GLN
1	D	477	THR
1	D	489	PHE
1	D	520	ARG
1	E	393	GLU
1	E	428	ARG
1	E	430	LYS
1	E	467	ASP
1	E	468	HIS
1	E	477	THR
1	E	489	PHE
1	E	490	ASN
1	E	518	HIS
1	E	520	ARG
1	F	395	VAL
1	F	400	GLN
1	F	402	GLN
1	F	428	ARG
1	F	467	ASP
1	F	477	THR
1	F	489	PHE
1	F	494	SER
1	F	518	HIS
1	F	520	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	GLN
1	A	468	HIS
1	B	398	GLN
1	B	446	HIS
1	B	475	GLN
1	C	505	ASN
1	E	475	GLN
1	E	508	HIS
1	E	522	GLN
1	F	400	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	151/160 (94%)	1.76	51 (33%)	0 0	69, 119, 172, 197	0
1	B	151/160 (94%)	1.87	53 (35%)	0 0	73, 118, 165, 219	0
1	C	151/160 (94%)	1.93	57 (37%)	0 0	74, 119, 164, 200	0
1	D	151/160 (94%)	2.16	57 (37%)	0 0	72, 119, 167, 202	0
1	E	151/160 (94%)	1.98	60 (39%)	0 0	77, 120, 167, 224	0
1	F	151/160 (94%)	1.98	61 (40%)	0 0	72, 114, 175, 218	0
All	All	906/960 (94%)	1.95	339 (37%)	0 0	69, 119, 169, 224	0

All (339) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	449	SER	13.1
1	D	537	LYS	11.7
1	C	468	HIS	10.8
1	D	472	LEU	9.5
1	E	472	LEU	9.4
1	C	482	ARG	9.3
1	D	482	ARG	9.2
1	D	445	ALA	8.6
1	F	497	PHE	8.5
1	F	482	ARG	8.4
1	F	448	ALA	8.2
1	D	512	GLU	7.6
1	C	446	HIS	7.6
1	B	472	LEU	7.4
1	B	417	LYS	7.3
1	F	447	LEU	7.3
1	F	472	LEU	7.3
1	D	448	ALA	7.2
1	C	472	LEU	7.0

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Mol	Chain	Res	Type	RSRZ
1	B	480	ILE	7.0
1	B	512	GLU	6.9
1	A	459	LEU	6.9
1	E	534	TRP	6.8
1	E	459	LEU	6.8
1	E	480	ILE	6.8
1	F	469	TRP	6.8
1	B	447	LEU	6.8
1	D	424	TYR	6.8
1	B	470	ILE	6.7
1	B	481	TRP	6.7
1	F	471	GLY	6.7
1	A	434	ARG	6.6
1	B	482	ARG	6.6
1	B	408	VAL	6.5
1	A	455	GLU	6.5
1	B	424	TYR	6.4
1	E	477	THR	6.4
1	C	469	TRP	6.4
1	A	526	MET	6.3
1	C	471	GLY	6.3
1	D	447	LEU	6.2
1	F	456	GLN	6.1
1	E	446	HIS	6.0
1	E	451	THR	6.0
1	C	470	ILE	6.0
1	B	534	TRP	6.0
1	F	460	VAL	6.0
1	C	532	TYR	5.9
1	D	498	TRP	5.9
1	D	497	PHE	5.8
1	F	530	SER	5.8
1	E	471	GLY	5.7
1	B	465	SER	5.6
1	C	481	TRP	5.6
1	E	400	GLN	5.5
1	E	455	GLU	5.5
1	D	523	TRP	5.5
1	E	482	ARG	5.4
1	C	485	ASP	5.4
1	F	434	ARG	5.4
1	D	446	HIS	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	433	TRP	5.4
1	A	472	LEU	5.3
1	B	471	GLY	5.2
1	D	481	TRP	5.2
1	A	516	CYS	5.2
1	F	470	ILE	5.2
1	F	532	TYR	5.2
1	D	471	GLY	5.2
1	E	449	SER	5.2
1	A	449	SER	5.1
1	B	448	ALA	5.1
1	B	436	ALA	5.1
1	F	433	TRP	5.1
1	B	498	TRP	5.1
1	D	423	PHE	5.1
1	C	530	SER	5.0
1	F	531	SER	5.0
1	B	423	PHE	5.0
1	A	500	LYS	5.0
1	E	511	GLY	5.0
1	B	523	TRP	5.0
1	F	449	SER	4.9
1	A	506	TRP	4.9
1	E	506	TRP	4.9
1	E	493	GLN	4.9
1	D	466	GLY	4.9
1	A	484	VAL	4.8
1	A	439	PHE	4.8
1	D	511	GLY	4.8
1	C	447	LEU	4.8
1	C	423	PHE	4.7
1	E	513	ARG	4.7
1	F	524	ASN	4.7
1	C	484	VAL	4.7
1	F	512	GLU	4.7
1	A	424	TYR	4.6
1	A	426	PHE	4.6
1	D	506	TRP	4.6
1	C	533	PRO	4.6
1	C	526	MET	4.6
1	D	538	LYS	4.6
1	E	501	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	513	ARG	4.5
1	C	402	GLN	4.5
1	E	517	VAL	4.5
1	E	417	LYS	4.5
1	D	412	ILE	4.5
1	D	408	VAL	4.5
1	C	512	GLU	4.4
1	E	494	SER	4.4
1	A	517	VAL	4.4
1	E	535	VAL	4.4
1	A	534	TRP	4.3
1	B	506	TRP	4.3
1	E	483	TRP	4.3
1	F	516	CYS	4.3
1	D	469	TRP	4.3
1	F	407	GLN	4.3
1	B	446	HIS	4.2
1	A	412	ILE	4.2
1	D	463	THR	4.2
1	F	484	VAL	4.2
1	D	516	CYS	4.2
1	D	459	LEU	4.2
1	A	468	HIS	4.1
1	B	439	PHE	4.0
1	D	508	HIS	4.0
1	E	542	TRP	4.0
1	D	460	VAL	4.0
1	D	483	TRP	4.0
1	E	532	TYR	4.0
1	C	439	PHE	4.0
1	E	426	PHE	3.9
1	D	434	ARG	3.9
1	F	423	PHE	3.9
1	C	435	GLU	3.8
1	E	434	ARG	3.8
1	D	450	VAL	3.8
1	A	470	ILE	3.8
1	C	527	ALA	3.8
1	B	503	PRO	3.8
1	A	523	TRP	3.8
1	F	473	THR	3.7
1	C	455	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	398	GLN	3.7
1	B	435	GLU	3.7
1	E	469	TRP	3.7
1	E	481	TRP	3.7
1	B	473	THR	3.7
1	A	481	TRP	3.6
1	C	483	TRP	3.6
1	F	526	MET	3.6
1	A	436	ALA	3.6
1	A	535	VAL	3.6
1	D	407	GLN	3.6
1	A	532	TYR	3.5
1	C	516	CYS	3.5
1	F	451	THR	3.5
1	D	399	LYS	3.5
1	F	419	PHE	3.5
1	B	532	TYR	3.5
1	E	436	ALA	3.5
1	E	484	VAL	3.5
1	D	501	ASN	3.4
1	F	435	GLU	3.4
1	C	451	THR	3.4
1	B	454	GLU	3.3
1	F	487	THR	3.3
1	A	469	TRP	3.3
1	E	412	ILE	3.3
1	A	430	LYS	3.3
1	C	458	PHE	3.3
1	E	523	TRP	3.2
1	F	511	GLY	3.2
1	B	509	ARG	3.2
1	F	537	LYS	3.2
1	D	436	ALA	3.2
1	D	527	ALA	3.2
1	C	408	VAL	3.2
1	C	424	TYR	3.1
1	E	470	ILE	3.1
1	A	446	HIS	3.1
1	B	537	LYS	3.1
1	D	451	THR	3.1
1	A	512	GLU	3.1
1	D	500	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	500	LYS	3.1
1	A	483	TRP	3.1
1	E	526	MET	3.0
1	C	459	LEU	3.0
1	A	513	ARG	3.0
1	F	409	LEU	3.0
1	D	534	TRP	3.0
1	B	412	ILE	3.0
1	A	407	GLN	3.0
1	C	419	PHE	3.0
1	E	435	GLU	3.0
1	F	411	LEU	3.0
1	E	498	TRP	2.9
1	B	507	ARG	2.9
1	C	462	THR	2.9
1	A	395	VAL	2.9
1	C	431	LYS	2.9
1	E	519	VAL	2.9
1	F	523	TRP	2.9
1	A	398	GLN	2.9
1	B	451	THR	2.9
1	F	517	VAL	2.9
1	B	433	TRP	2.9
1	C	534	TRP	2.9
1	C	517	VAL	2.9
1	C	448	ALA	2.8
1	D	456	GLN	2.8
1	C	487	THR	2.8
1	F	425	TYR	2.8
1	F	518	HIS	2.8
1	E	439	PHE	2.8
1	D	517	VAL	2.8
1	E	425	TYR	2.8
1	F	507	ARG	2.8
1	A	419	PHE	2.8
1	C	511	GLY	2.8
1	E	456	GLN	2.8
1	A	498	TRP	2.8
1	E	415	ASN	2.8
1	D	433	TRP	2.8
1	B	500	LYS	2.8
1	B	449	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	423	PHE	2.7
1	D	470	ILE	2.7
1	A	511	GLY	2.7
1	E	479	GLY	2.7
1	B	406	ASN	2.7
1	F	542	TRP	2.7
1	F	408	VAL	2.7
1	F	481	TRP	2.7
1	A	408	VAL	2.6
1	F	489	PHE	2.6
1	F	506	TRP	2.6
1	B	484	VAL	2.6
1	F	439	PHE	2.6
1	D	487	THR	2.6
1	E	407	GLN	2.6
1	D	444	GLY	2.6
1	F	498	TRP	2.6
1	A	527	ALA	2.6
1	B	459	LEU	2.6
1	C	518	HIS	2.6
1	C	398	GLN	2.6
1	E	475	GLN	2.6
1	D	435	GLU	2.6
1	C	488	PRO	2.6
1	C	542	TRP	2.6
1	E	487	THR	2.6
1	B	399	LYS	2.6
1	F	533	PRO	2.5
1	F	395	VAL	2.5
1	F	455	GLU	2.5
1	C	399	LYS	2.5
1	B	469	TRP	2.5
1	F	508	HIS	2.5
1	B	511	GLY	2.5
1	D	480	ILE	2.5
1	C	436	ALA	2.5
1	F	445	ALA	2.5
1	B	437	GLU	2.5
1	F	458	PHE	2.5
1	D	473	THR	2.5
1	E	512	GLU	2.5
1	F	527	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	405	GLN	2.4
1	A	462	THR	2.4
1	C	460	VAL	2.4
1	D	485	ASP	2.4
1	F	462	THR	2.4
1	B	488	PRO	2.4
1	D	513	ARG	2.4
1	E	405	GLN	2.4
1	B	543	SER	2.4
1	A	417	LYS	2.4
1	E	430	LYS	2.4
1	F	500	LYS	2.4
1	C	400	GLN	2.4
1	F	446	HIS	2.4
1	C	437	GLU	2.4
1	F	483	TRP	2.4
1	B	526	MET	2.3
1	B	477	THR	2.3
1	C	411	LEU	2.3
1	B	519	VAL	2.3
1	B	426	PHE	2.3
1	C	426	PHE	2.3
1	C	498	TRP	2.3
1	E	473	THR	2.3
1	E	438	LYS	2.3
1	E	433	TRP	2.3
1	F	454	GLU	2.3
1	E	424	TYR	2.3
1	A	475	GLN	2.3
1	A	448	ALA	2.3
1	B	487	THR	2.3
1	A	445	ALA	2.3
1	E	408	VAL	2.3
1	A	537	LYS	2.2
1	C	395	VAL	2.2
1	C	509	ARG	2.2
1	C	519	VAL	2.2
1	D	428	ARG	2.2
1	F	394	ALA	2.2
1	C	528	CYS	2.2
1	A	487	THR	2.2
1	D	507	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	534	TRP	2.2
1	A	451	THR	2.2
1	B	517	VAL	2.1
1	B	415	ASN	2.1
1	B	531	SER	2.1
1	B	418	TYR	2.1
1	A	438	LYS	2.1
1	C	467	ASP	2.1
1	C	473	THR	2.1
1	B	464	SER	2.1
1	E	497	PHE	2.1
1	D	535	VAL	2.1
1	E	533	PRO	2.1
1	A	471	GLY	2.1
1	D	454	GLU	2.1
1	D	519	VAL	2.1
1	E	395	VAL	2.1
1	F	424	TYR	2.1
1	A	465	SER	2.1
1	C	500	LYS	2.0
1	D	453	GLN	2.0
1	A	507	ARG	2.0
1	D	427	SER	2.0
1	E	485	ASP	2.0
1	F	485	ASP	2.0
1	E	409	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	D	602	1/1	0.47	0.19	114,114,114,114	0
2	CA	C	602	1/1	0.62	0.17	107,107,107,107	0
2	CA	B	602	1/1	0.66	0.11	132,132,132,132	0
2	CA	F	601	1/1	0.67	0.24	108,108,108,108	0
2	CA	F	602	1/1	0.67	0.30	122,122,122,122	0
2	CA	D	601	1/1	0.76	0.24	105,105,105,105	0
2	CA	C	601	1/1	0.78	0.17	98,98,98,98	0
2	CA	E	602	1/1	0.84	0.12	105,105,105,105	0
2	CA	A	602	1/1	0.89	0.18	101,101,101,101	0
2	CA	A	601	1/1	0.91	0.11	110,110,110,110	0
2	CA	B	601	1/1	0.94	0.30	102,102,102,102	0
2	CA	E	601	1/1	0.97	0.20	102,102,102,102	0

6.5 Other polymers (i)

There are no such residues in this entry.