Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:00 AM GMT

PDB ID	:	2VKX
Title	:	HUMAN NCAM, FN3 DOMAINS 1 AND 2, M610R MUTANT
Authors	:	Carafoli, F.; Saffell, J.L.; Hohenester, E.
Deposited on	:	2008-01-04
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

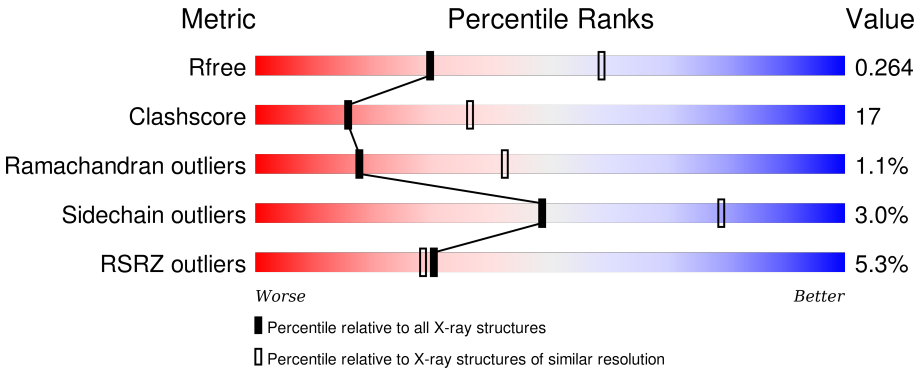
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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. 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	209	% 68% 25% • 5%
1	B	209	3% 71% 22% • 5%
1	C	209	6% 62% 31% • 5%
1	D	209	9% 64% 29% • 5%
1	E	209	4% 72% 24% • •

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Mol	Chain	Length	Quality of chain
1	F	209	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9350 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.

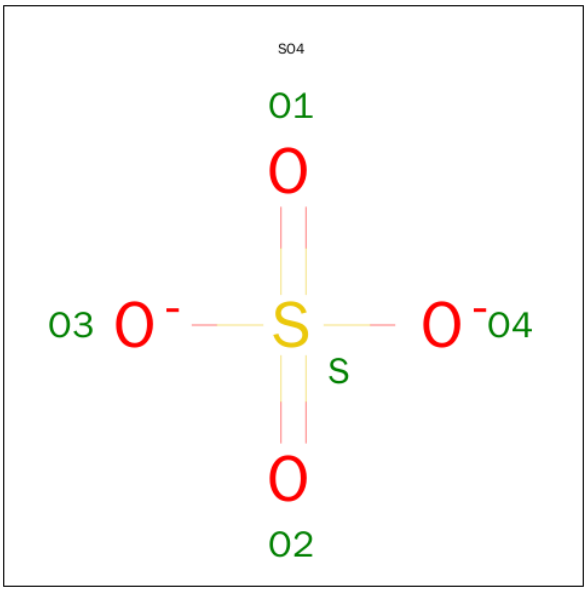
- Molecule 1 is a protein called NEURAL CELL ADHESION MOLECULE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	1
			1540	971	266	301	2			
1	B	198	Total	C	N	O	S	0	0	1
			1535	968	265	300	2			
1	C	199	Total	C	N	O	S	0	0	1
			1540	971	266	301	2			
1	D	199	Total	C	N	O	S	0	0	1
			1540	971	266	301	2			
1	E	203	Total	C	N	O	S	0	0	1
			1569	990	271	306	2			
1	F	199	Total	C	N	O	S	0	0	1
			1540	971	266	301	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	610	ARG	MET	ENGINEERED MUTATION	UNP P13591
B	610	ARG	MET	ENGINEERED MUTATION	UNP P13591
C	610	ARG	MET	ENGINEERED MUTATION	UNP P13591
D	610	ARG	MET	ENGINEERED MUTATION	UNP P13591
E	610	ARG	MET	ENGINEERED MUTATION	UNP P13591
F	610	ARG	MET	ENGINEERED MUTATION	UNP P13591

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

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

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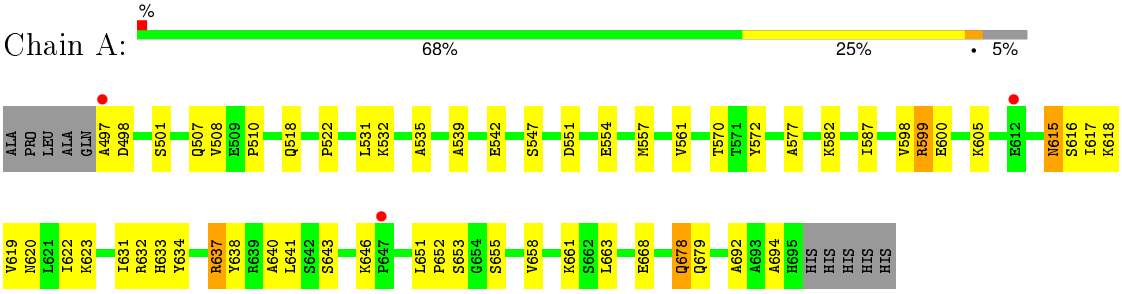
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	6	Total O 6 6	0	0
3	C	7	Total O 7 7	0	0
3	D	5	Total O 5 5	0	0
3	E	5	Total O 5 5	0	0
3	F	5	Total O 5 5	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

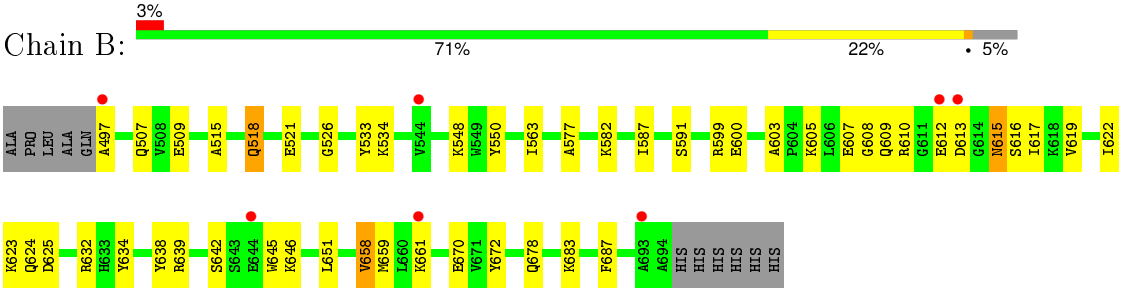
- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain A:



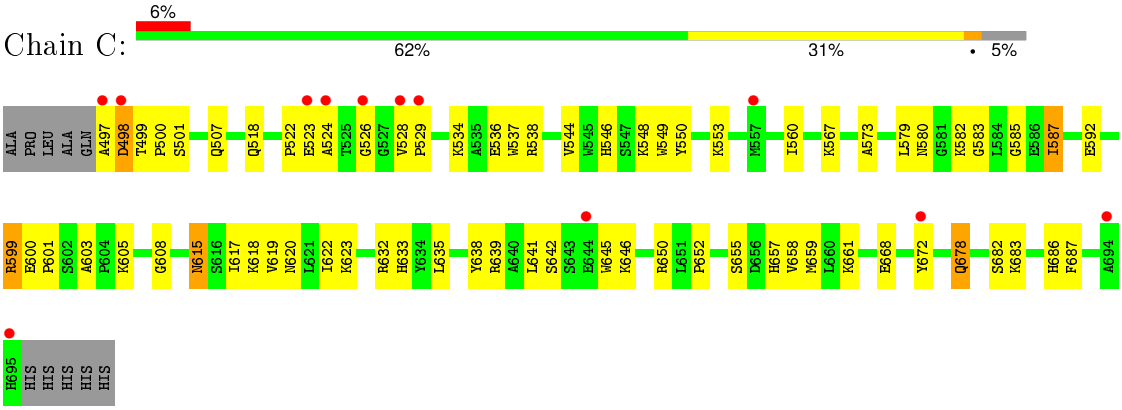
- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain B:



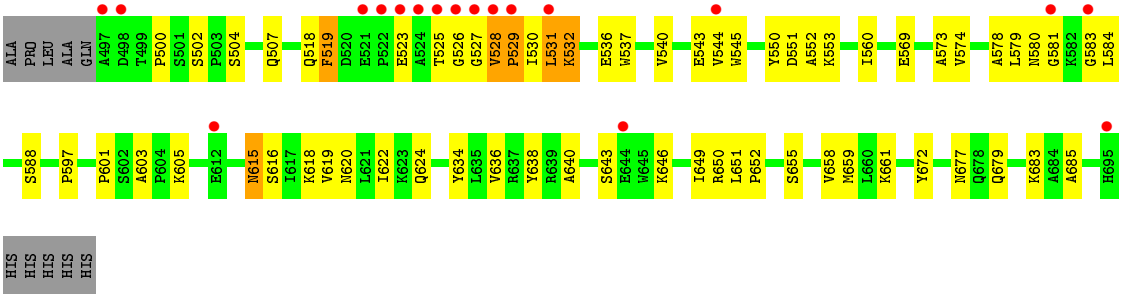
- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain C:

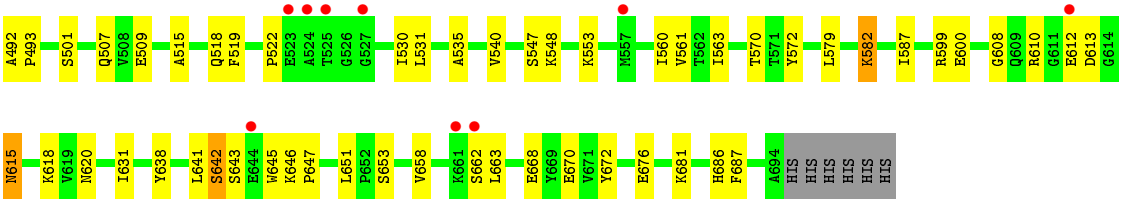


- Molecule 1: NEURAL CELL ADHESION MOLECULE

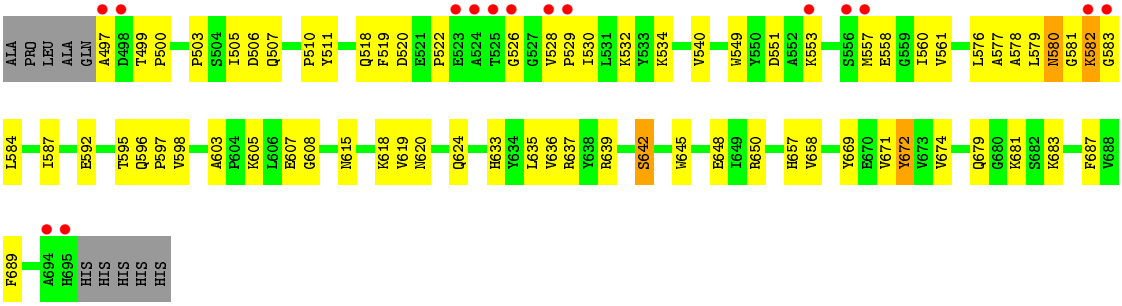
Chain D:



• Molecule 1: NEURAL CELL ADHESION MOLECULE



• Molecule 1: NEURAL CELL ADHESION MOLECULE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.42Å 107.57Å 161.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.70) 99.2 (19.97-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.268 0.219 , 0.264	Depositor DCC
R_{free} test set	2227 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 44346 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9350	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.42	0/1577	0.65	0/2141
1	B	0.40	0/1572	0.64	0/2134
1	C	0.40	0/1577	0.62	0/2141
1	D	0.37	0/1577	0.63	0/2141
1	E	0.38	0/1607	0.64	0/2183
1	F	0.37	0/1577	0.64	0/2141
All	All	0.39	0/9487	0.64	0/12881

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	1540	0	1501	45	0
1	B	1535	0	1496	47	0
1	C	1540	0	1501	61	0
1	D	1540	0	1501	57	0
1	E	1569	0	1532	52	0
1	F	1540	0	1501	64	0
2	A	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	25	0	0	0	0
3	A	3	0	0	0	0
3	B	6	0	0	0	0
3	C	7	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
All	All	9350	0	9032	313	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 17.

All (313) 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:507:GLN:HB2	1:E:518:GLN:HB2	1.50	0.94
1:D:615:ASN:H	1:D:615:ASN:HD22	1.20	0.89
1:D:518:GLN:HG2	1:D:560:ILE:HG22	1.59	0.84
1:B:619:VAL:HB	1:B:658:VAL:HG13	1.60	0.82
1:C:615:ASN:HD22	1:C:615:ASN:H	1.33	0.76
1:B:599:ARG:HE	1:B:600:GLU:H	1.31	0.75
1:D:507:GLN:HB2	1:D:518:GLN:HB2	1.67	0.74
1:B:615:ASN:HD22	1:B:615:ASN:H	1.35	0.73
1:E:492:ALA:N	1:E:493:PRO:HD2	2.03	0.73
1:C:599:ARG:NE	1:C:600:GLU:H	1.87	0.72
1:F:503:PRO:HG3	1:F:522:PRO:HG3	1.73	0.71
1:A:507:GLN:HB2	1:A:518:GLN:HB2	1.72	0.71
1:D:618:LYS:NZ	1:D:620:ASN:HD21	1.89	0.71
1:B:605:LYS:HG3	1:B:624:GLN:NE2	2.05	0.71
1:E:599:ARG:HG3	1:E:600:GLU:N	2.05	0.70
1:E:553:LYS:HB2	1:E:553:LYS:NZ	2.06	0.70
1:F:619:VAL:HB	1:F:658:VAL:CG1	2.21	0.70
1:F:551:ASP:OD2	1:F:553:LYS:HB3	1.92	0.69
1:F:532:LYS:HD3	1:F:551:ASP:HA	1.73	0.69
1:C:659:MET:HG2	1:C:661:LYS:HE2	1.73	0.69
1:C:528:VAL:HB	1:C:529:PRO:HD2	1.76	0.68
1:A:539:ALA:HB3	1:A:542:GLU:HG2	1.75	0.67
1:A:531:LEU:O	1:A:532:LYS:HD3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ARG:NE	1:A:600:GLU:H	1.93	0.67
1:E:618:LYS:HE2	1:E:620:ASN:HD21	1.60	0.66
1:C:507:GLN:HB2	1:C:518:GLN:HB2	1.77	0.66
1:F:605:LYS:HG3	1:F:624:GLN:NE2	2.10	0.66
1:F:522:PRO:HG2	1:F:578:ALA:CB	2.24	0.66
1:C:605:LYS:HB2	1:C:622:ILE:HB	1.76	0.66
1:D:605:LYS:HE2	1:D:624:GLN:HE22	1.61	0.65
1:C:599:ARG:HG3	1:C:600:GLU:N	2.11	0.65
1:E:599:ARG:NE	1:E:600:GLU:HG3	2.11	0.65
1:A:577:ALA:HB2	1:A:587:ILE:HG22	1.79	0.65
1:D:605:LYS:HB2	1:D:622:ILE:HB	1.79	0.65
1:D:500:PRO:HB2	1:D:578:ALA:HB3	1.78	0.65
1:A:652:PRO:HD2	1:A:655:SER:OG	1.97	0.64
1:A:632:ARG:HG2	1:A:633:HIS:CD2	2.32	0.64
1:E:518:GLN:HG3	1:E:560:ILE:CG2	2.27	0.64
1:D:529:PRO:O	1:D:580:ASN:HB3	1.96	0.64
1:F:619:VAL:HB	1:F:658:VAL:HG13	1.77	0.64
1:A:618:LYS:HE2	1:A:620:ASN:HD21	1.61	0.64
1:F:507:GLN:HB2	1:F:518:GLN:HB3	1.79	0.64
1:A:618:LYS:HE2	1:A:620:ASN:ND2	2.13	0.63
1:C:497:ALA:HA	1:C:526:GLY:O	1.99	0.63
1:B:632:ARG:HD2	1:B:678:GLN:NE2	2.14	0.63
1:A:599:ARG:HE	1:A:600:GLU:H	1.46	0.62
1:D:532:LYS:HA	1:D:550:TYR:O	1.99	0.62
1:D:634:TYR:HB2	1:D:651:LEU:HB2	1.81	0.62
1:E:599:ARG:HG3	1:E:600:GLU:H	1.65	0.62
1:B:610:ARG:HE	1:E:610:ARG:HD3	1.66	0.61
1:B:497:ALA:HB1	1:B:582:LYS:NZ	2.15	0.61
1:A:542:GLU:OE2	1:A:542:GLU:HA	2.01	0.61
1:F:532:LYS:NZ	1:F:551:ASP:HB2	2.14	0.61
1:C:501:SER:HB3	1:C:524:ALA:HB3	1.81	0.61
1:F:549:TRP:HH2	1:F:584:LEU:HD13	1.65	0.61
1:B:507:GLN:HB2	1:B:518:GLN:HB2	1.83	0.60
1:C:599:ARG:HE	1:C:600:GLU:H	1.48	0.60
1:D:519:PHE:N	1:D:519:PHE:CD2	2.68	0.60
1:D:525:THR:HG21	1:D:530:ILE:HG12	1.84	0.60
1:B:610:ARG:NE	1:E:610:ARG:HD3	2.17	0.60
1:F:499:THR:HG22	1:F:583:GLY:H	1.67	0.60
1:E:615:ASN:HB2	1:E:663:LEU:O	2.01	0.60
1:C:639:ARG:HD3	1:C:645:TRP:CD2	2.37	0.59
1:E:641:LEU:O	1:E:642:SER:CB	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:LYS:HG3	1:B:624:GLN:HE21	1.67	0.59
1:F:618:LYS:NZ	1:F:620:ASN:HD21	2.00	0.59
1:D:601:PRO:HD3	1:D:677:ASN:ND2	2.17	0.59
1:D:531:LEU:HD23	1:D:531:LEU:N	2.18	0.59
1:F:500:PRO:HD3	1:F:580:ASN:CG	2.23	0.59
1:D:618:LYS:HZ2	1:D:620:ASN:HD21	1.51	0.59
1:F:534:LYS:HD2	1:F:584:LEU:HD21	1.85	0.59
1:C:553:LYS:HB2	1:C:553:LYS:NZ	2.17	0.59
1:C:518:GLN:HG3	1:C:560:ILE:HG22	1.85	0.59
1:F:497:ALA:HB1	1:F:526:GLY:O	2.02	0.59
1:D:532:LYS:HD3	1:D:551:ASP:HA	1.84	0.58
1:E:599:ARG:HE	1:E:600:GLU:H	1.50	0.58
1:D:579:LEU:HG	1:D:583:GLY:O	2.04	0.57
1:F:577:ALA:HB2	1:F:587:ILE:HG22	1.87	0.57
1:D:569:GLU:CG	1:D:597:PRO:HB3	2.35	0.57
1:B:659:MET:HG2	1:B:661:LYS:HE3	1.87	0.57
1:D:531:LEU:HD23	1:D:531:LEU:H	1.70	0.57
1:A:692:ALA:HB1	2:A:1697:SO4:O2	2.05	0.57
1:D:528:VAL:N	1:D:529:PRO:CD	2.68	0.56
1:F:639:ARG:HD3	1:F:645:TRP:CE3	2.40	0.56
1:C:638:TYR:CZ	1:C:646:LYS:HG3	2.40	0.56
1:D:528:VAL:N	1:D:529:PRO:HD3	2.21	0.55
1:D:519:PHE:HD2	1:D:519:PHE:N	2.03	0.55
1:E:553:LYS:HZ2	1:E:553:LYS:HB2	1.70	0.55
1:D:500:PRO:HD3	1:D:580:ASN:ND2	2.22	0.55
1:E:492:ALA:N	1:E:493:PRO:CD	2.68	0.55
1:E:519:PHE:HE2	1:E:561:VAL:HG13	1.71	0.55
1:E:518:GLN:HG3	1:E:560:ILE:HG22	1.88	0.55
1:D:615:ASN:N	1:D:615:ASN:HD22	1.92	0.54
1:A:501:SER:O	1:A:522:PRO:HB3	2.07	0.54
1:B:497:ALA:HA	1:B:526:GLY:HA2	1.90	0.54
1:D:640:ALA:HB3	1:D:643:SER:HB3	1.89	0.54
1:E:670:GLU:HB2	1:E:686:HIS:CE1	2.43	0.54
1:C:560:ILE:HD12	1:C:560:ILE:C	2.28	0.54
1:E:599:ARG:CG	1:E:600:GLU:N	2.71	0.53
1:C:632:ARG:HG2	1:C:633:HIS:CD2	2.43	0.53
1:B:599:ARG:HH21	1:B:600:GLU:HG3	1.74	0.53
1:C:522:PRO:C	1:C:524:ALA:H	2.12	0.53
1:C:548:LYS:HD3	1:C:550:TYR:OH	2.08	0.53
1:A:605:LYS:HB2	1:A:622:ILE:HB	1.90	0.53
1:B:623:LYS:O	1:B:624:GLN:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:599:ARG:NE	1:E:600:GLU:H	2.06	0.53
1:C:639:ARG:HB3	1:C:645:TRP:HA	1.90	0.53
1:A:617:ILE:HG12	1:A:618:LYS:N	2.24	0.53
1:F:637:ARG:HG2	1:F:648:GLU:HA	1.90	0.53
1:B:610:ARG:CZ	1:E:610:ARG:HH11	2.22	0.52
1:B:515:ALA:HB3	1:B:563:ILE:HD11	1.91	0.52
1:D:619:VAL:HB	1:D:658:VAL:CG1	2.40	0.52
1:D:540:VAL:O	1:F:642:SER:HB3	2.09	0.52
1:A:507:GLN:HB2	1:A:518:GLN:CB	2.36	0.52
1:B:509:GLU:OE1	1:B:509:GLU:HA	2.09	0.52
1:C:599:ARG:HH21	1:C:600:GLU:HG3	1.73	0.52
1:D:651:LEU:HD11	1:D:658:VAL:HB	1.92	0.52
1:A:599:ARG:HE	1:A:599:ARG:HA	1.74	0.52
1:E:612:GLU:HG3	1:E:613:ASP:OD2	2.09	0.52
1:C:620:ASN:ND2	1:C:657:HIS:ND1	2.58	0.52
1:B:634:TYR:HB2	1:B:651:LEU:HB2	1.92	0.52
1:E:599:ARG:CG	1:E:600:GLU:H	2.22	0.52
1:D:500:PRO:HD3	1:D:580:ASN:CG	2.31	0.51
1:D:544:VAL:HG12	1:D:545:TRP:N	2.25	0.51
1:F:608:GLY:HA3	1:F:687:PHE:CZ	2.45	0.51
1:E:560:ILE:HD12	1:E:560:ILE:O	2.09	0.51
1:B:534:LYS:HB3	1:B:577:ALA:HB3	1.91	0.51
1:E:599:ARG:HE	1:E:600:GLU:N	2.09	0.51
1:C:652:PRO:HD2	1:C:655:SER:OG	2.11	0.51
1:C:615:ASN:HD22	1:C:615:ASN:N	1.99	0.51
1:D:527:GLY:C	1:D:528:VAL:HG23	2.31	0.51
1:C:499:THR:HB	1:C:585:GLY:HA2	1.92	0.51
1:B:612:GLU:HG3	1:B:613:ASP:N	2.27	0.50
1:D:636:VAL:HB	1:D:649:ILE:HB	1.94	0.50
1:C:617:ILE:HG12	1:C:618:LYS:N	2.27	0.50
1:E:608:GLY:HA3	1:E:687:PHE:CZ	2.46	0.50
1:C:518:GLN:CG	1:C:560:ILE:HG22	2.42	0.50
1:B:599:ARG:NE	1:B:600:GLU:H	2.02	0.50
1:C:498:ASP:HA	1:C:582:LYS:HE2	1.93	0.50
1:D:619:VAL:HB	1:D:658:VAL:HG13	1.94	0.50
1:F:633:HIS:CE1	1:F:650:ARG:HH21	2.30	0.50
1:F:636:VAL:HG11	1:F:658:VAL:HG21	1.93	0.49
1:F:499:THR:HG22	1:F:582:LYS:HB2	1.94	0.49
1:F:519:PHE:HE2	1:F:561:VAL:HG13	1.76	0.49
1:E:531:LEU:HB2	1:E:579:LEU:HD23	1.94	0.49
1:F:579:LEU:HB2	1:F:584:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:620:ASN:ND2	1:F:657:HIS:ND1	2.60	0.49
1:F:532:LYS:HZ3	1:F:551:ASP:HB2	1.76	0.49
1:A:631:ILE:O	1:A:653:SER:HB3	2.12	0.49
1:F:528:VAL:HG11	1:F:581:GLY:HA3	1.93	0.49
1:F:534:LYS:HB2	1:F:549:TRP:CZ3	2.48	0.49
1:E:645:TRP:HH2	1:E:672:TYR:CD1	2.30	0.49
1:B:612:GLU:HG2	1:B:661:LYS:HE2	1.95	0.48
1:A:637:ARG:HG3	1:A:637:ARG:NH1	2.26	0.48
1:C:537:TRP:HA	1:C:573:ALA:O	2.14	0.48
1:A:599:ARG:HE	1:A:600:GLU:N	2.11	0.48
1:C:603:ALA:HB2	1:C:683:LYS:O	2.14	0.48
1:C:501:SER:O	1:C:522:PRO:HB3	2.12	0.48
1:E:641:LEU:O	1:E:642:SER:HB3	2.14	0.48
1:E:670:GLU:HB2	1:E:686:HIS:HE1	1.79	0.48
1:F:522:PRO:HD2	1:F:530:ILE:HD13	1.96	0.47
1:D:537:TRP:HA	1:D:573:ALA:O	2.14	0.47
1:A:554:GLU:OE2	1:B:550:TYR:HA	2.14	0.47
1:D:605:LYS:HE2	1:D:624:GLN:NE2	2.26	0.47
1:F:534:LYS:CD	1:F:584:LEU:HD21	2.45	0.47
1:C:641:LEU:O	1:C:642:SER:OG	2.32	0.47
1:F:674:VAL:HG11	1:F:681:LYS:HB3	1.96	0.47
1:E:515:ALA:HB3	1:E:563:ILE:HG12	1.96	0.47
1:D:519:PHE:HD2	1:D:519:PHE:H	1.61	0.47
1:B:612:GLU:OE2	1:B:661:LYS:HD3	2.15	0.47
1:D:536:GLU:O	1:D:574:VAL:HA	2.15	0.47
1:C:534:LYS:HB2	1:C:549:TRP:CZ3	2.50	0.47
1:C:528:VAL:HG23	1:C:580:ASN:HB2	1.97	0.47
1:E:615:ASN:OD1	1:E:662:SER:HA	2.15	0.47
1:A:678:GLN:H	1:A:678:GLN:HG2	1.50	0.47
1:B:607:GLU:OE1	1:E:668:GLU:OE1	2.33	0.47
1:A:599:ARG:HG3	1:A:600:GLU:N	2.29	0.47
1:B:638:TYR:CZ	1:B:646:LYS:HG3	2.49	0.46
1:C:638:TYR:CE1	1:C:646:LYS:HG3	2.50	0.46
1:B:632:ARG:HD2	1:B:678:GLN:HE22	1.78	0.46
1:A:598:VAL:HG23	1:A:679:GLN:OE1	2.15	0.46
1:F:540:VAL:HG21	1:F:592:GLU:OE2	2.16	0.46
1:D:652:PRO:HD2	1:D:655:SER:OG	2.16	0.46
1:D:527:GLY:C	1:D:529:PRO:HD3	2.35	0.46
1:E:548:LYS:HE2	1:F:557:MET:HB3	1.97	0.46
1:F:506:ASP:OD2	1:F:520:ASP:OD2	2.33	0.46
1:E:615:ASN:H	1:E:615:ASN:HD22	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:VAL:O	1:A:510:PRO:HD3	2.16	0.46
1:E:638:TYR:CE1	1:E:646:LYS:HG3	2.50	0.46
1:F:596:GLN:HB3	1:F:597:PRO:HD2	1.97	0.46
1:C:599:ARG:CG	1:C:600:GLU:N	2.77	0.46
1:A:599:ARG:CA	1:A:599:ARG:HE	2.29	0.45
1:A:561:VAL:O	1:A:561:VAL:HG23	2.16	0.45
1:C:599:ARG:HG3	1:C:600:GLU:O	2.15	0.45
1:A:539:ALA:HB3	1:A:542:GLU:CG	2.45	0.45
1:E:676:GLU:HG3	1:E:681:LYS:HG2	1.98	0.45
1:D:615:ASN:N	1:D:615:ASN:ND2	2.63	0.45
1:B:645:TRP:HH2	1:B:672:TYR:CE1	2.34	0.45
1:E:501:SER:O	1:E:522:PRO:HB3	2.16	0.45
1:B:616:SER:HB2	1:B:661:LYS:HG2	1.98	0.45
1:B:645:TRP:HH2	1:B:672:TYR:CD1	2.33	0.45
1:E:582:LYS:N	1:E:582:LYS:HD2	2.30	0.45
1:B:659:MET:CG	1:B:661:LYS:HE3	2.46	0.45
1:C:579:LEU:HD12	1:C:583:GLY:C	2.37	0.45
1:B:608:GLY:HA3	1:B:687:PHE:CZ	2.51	0.45
1:E:570:THR:HB	1:E:572:TYR:CE2	2.52	0.45
1:F:532:LYS:HZ2	1:F:551:ASP:HB2	1.80	0.45
1:C:587:ILE:HG12	1:C:587:ILE:H	1.50	0.45
1:D:502:SER:HB2	1:D:588:SER:HA	1.99	0.45
1:D:531:LEU:CD2	1:D:580:ASN:HA	2.47	0.45
1:C:617:ILE:HD11	1:C:687:PHE:CE2	2.52	0.45
1:C:659:MET:HG2	1:C:661:LYS:CE	2.45	0.45
1:C:497:ALA:C	1:C:582:LYS:HE2	2.37	0.45
1:C:601:PRO:HG2	1:C:682:SER:HB3	1.98	0.45
1:D:532:LYS:N	1:D:552:ALA:HB2	2.32	0.44
1:E:515:ALA:HB3	1:E:563:ILE:CG1	2.46	0.44
1:C:619:VAL:HB	1:C:658:VAL:CG1	2.48	0.44
1:F:522:PRO:HD2	1:F:530:ILE:CD1	2.46	0.44
1:F:618:LYS:HZ2	1:F:620:ASN:HD21	1.65	0.44
1:D:579:LEU:HB2	1:D:584:LEU:HD12	1.97	0.44
1:A:616:SER:HB2	1:A:661:LYS:HA	1.99	0.44
1:E:618:LYS:HE2	1:E:620:ASN:ND2	2.32	0.44
1:F:645:TRP:CH2	1:F:672:TYR:HB2	2.52	0.44
1:D:638:TYR:CE1	1:D:646:LYS:HG3	2.53	0.44
1:A:638:TYR:CE1	1:A:646:LYS:HG3	2.51	0.44
1:A:615:ASN:ND2	1:A:615:ASN:C	2.70	0.44
1:A:615:ASN:O	1:A:663:LEU:HB2	2.18	0.44
1:A:619:VAL:HB	1:A:658:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:510:PRO:HB2	1:F:595:THR:HA	1.99	0.44
1:A:557:MET:SD	1:B:548:LYS:HE2	2.58	0.44
1:C:553:LYS:HB2	1:C:553:LYS:HZ2	1.82	0.44
1:E:651:LEU:HD11	1:E:658:VAL:HB	1.99	0.44
1:C:678:GLN:H	1:C:678:GLN:HG2	1.59	0.44
1:E:509:GLU:OE1	1:E:509:GLU:HA	2.18	0.44
1:C:617:ILE:HD11	1:C:687:PHE:HE2	1.83	0.43
1:C:635:LEU:CD2	1:C:650:ARG:HG2	2.48	0.43
1:E:631:ILE:O	1:E:653:SER:HB3	2.17	0.43
1:F:528:VAL:HG11	1:F:581:GLY:CA	2.48	0.43
1:C:500:PRO:HG3	1:C:580:ASN:ND2	2.34	0.43
1:F:639:ARG:HD3	1:F:645:TRP:CZ3	2.53	0.43
1:D:618:LYS:HZ3	1:D:620:ASN:HD21	1.65	0.43
1:E:638:TYR:CZ	1:E:646:LYS:HG3	2.53	0.43
1:B:599:ARG:HG3	1:B:600:GLU:N	2.34	0.43
1:A:637:ARG:HH11	1:A:637:ARG:CG	2.32	0.43
1:D:523:GLU:O	1:D:523:GLU:HG2	2.17	0.43
1:F:560:ILE:O	1:F:560:ILE:HD12	2.18	0.43
1:D:649:ILE:HG22	1:D:650:ARG:N	2.33	0.43
1:A:557:MET:CE	1:B:548:LYS:HE2	2.49	0.43
1:B:623:LYS:C	1:B:624:GLN:HG2	2.39	0.43
1:E:646:LYS:HB3	1:E:647:PRO:CD	2.49	0.43
1:B:603:ALA:HB2	1:B:683:LYS:O	2.19	0.43
1:D:615:ASN:H	1:D:615:ASN:ND2	2.01	0.43
1:A:634:TYR:HB2	1:A:651:LEU:HB2	2.00	0.43
1:B:639:ARG:NH2	1:B:670:GLU:OE1	2.51	0.43
1:F:669:TYR:HB2	1:F:689:PHE:CZ	2.54	0.43
1:C:528:VAL:CG2	1:C:580:ASN:HB2	2.49	0.43
1:F:528:VAL:HA	1:F:529:PRO:HD3	1.86	0.43
1:E:599:ARG:CZ	1:E:600:GLU:HG3	2.49	0.42
1:D:672:TYR:HA	1:D:685:ALA:O	2.19	0.42
1:B:497:ALA:HB1	1:B:582:LYS:HZ3	1.82	0.42
1:C:615:ASN:H	1:C:615:ASN:ND2	2.09	0.42
1:E:530:ILE:HD12	1:E:530:ILE:N	2.34	0.42
1:C:567:LYS:HE2	2:C:1696:SO4:O3	2.19	0.42
1:F:560:ILE:HD12	1:F:560:ILE:C	2.39	0.42
1:C:672:TYR:CZ	1:C:686:HIS:CD2	3.08	0.42
1:B:521:GLU:HG2	1:B:533:TYR:OH	2.19	0.42
1:A:532:LYS:NZ	1:A:551:ASP:OD1	2.49	0.42
1:D:603:ALA:HB2	1:D:683:LYS:O	2.20	0.42
1:D:677:ASN:OD1	1:D:679:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:ALA:O	1:A:643:SER:HB3	2.19	0.42
1:B:605:LYS:HB2	1:B:622:ILE:HB	2.02	0.42
1:B:624:GLN:O	1:B:625:ASP:C	2.58	0.42
1:C:642:SER:OG	1:E:540:VAL:O	2.34	0.42
1:F:598:VAL:HG23	1:F:679:GLN:OE1	2.20	0.42
1:E:535:ALA:O	1:E:547:SER:HA	2.20	0.42
1:F:500:PRO:HD3	1:F:580:ASN:OD1	2.19	0.42
1:F:558:GLU:OE1	1:F:560:ILE:HD11	2.20	0.42
1:C:668:GLU:OE1	1:F:607:GLU:OE1	2.38	0.42
1:F:618:LYS:HZ3	1:F:620:ASN:HD21	1.67	0.41
1:E:658:VAL:HG13	1:E:658:VAL:O	2.20	0.41
1:C:536:GLU:HA	1:C:546:HIS:O	2.20	0.41
1:C:497:ALA:O	1:C:582:LYS:HE2	2.20	0.41
1:A:637:ARG:HH11	1:A:637:ARG:HG3	1.85	0.41
1:B:642:SER:OG	1:F:540:VAL:O	2.30	0.41
1:F:603:ALA:HB2	1:F:683:LYS:O	2.20	0.41
1:B:619:VAL:HB	1:B:658:VAL:CG1	2.41	0.41
1:F:582:LYS:HB2	1:F:583:GLY:H	1.70	0.41
1:C:618:LYS:HE2	1:C:620:ASN:HD21	1.85	0.41
1:A:615:ASN:HD22	1:A:615:ASN:C	2.24	0.41
1:D:504:SER:O	1:D:519:PHE:HA	2.20	0.41
1:C:608:GLY:HA3	1:C:687:PHE:CZ	2.55	0.41
1:F:637:ARG:HD3	1:F:648:GLU:HB2	2.02	0.41
1:B:638:TYR:CE1	1:B:646:LYS:HG3	2.55	0.41
1:A:668:GLU:OE1	1:C:592:GLU:OE2	2.38	0.41
1:F:580:ASN:HD22	1:F:580:ASN:H	1.68	0.41
1:C:658:VAL:HG13	1:C:658:VAL:O	2.21	0.41
1:F:683:LYS:H	1:F:683:LYS:HG2	1.71	0.41
1:B:609:GLN:O	1:B:617:ILE:HG13	2.20	0.41
1:D:659:MET:HG3	1:D:661:LYS:HG3	2.03	0.41
1:B:599:ARG:HG3	1:B:600:GLU:H	1.86	0.41
1:F:635:LEU:HB2	1:F:674:VAL:HB	2.03	0.40
1:F:580:ASN:HD22	1:F:580:ASN:N	2.18	0.40
1:A:497:ALA:O	1:A:582:LYS:HE2	2.20	0.40
1:F:511:TYR:O	1:F:595:THR:HB	2.21	0.40
1:A:570:THR:HB	1:A:572:TYR:CE2	2.56	0.40
1:F:505:ILE:HG12	1:F:576:LEU:HD12	2.03	0.40
1:D:569:GLU:HG3	1:D:597:PRO:HB3	2.03	0.40
1:F:674:VAL:CG1	1:F:681:LYS:HB3	2.52	0.40
1:D:616:SER:HB2	1:D:661:LYS:HG2	2.03	0.40
1:D:500:PRO:HG3	1:D:525:THR:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:SER:OG	1:C:522:PRO:HB2	2.22	0.40
1:F:671:VAL:HG12	1:F:672:TYR:N	2.36	0.40
1:A:535:ALA:O	1:A:547:SER:HA	2.22	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	197/209 (94%)	188 (95%)	7 (4%)	2 (1%)	19 45
1	B	196/209 (94%)	188 (96%)	8 (4%)	0	100 100
1	C	197/209 (94%)	188 (95%)	7 (4%)	2 (1%)	19 45
1	D	197/209 (94%)	177 (90%)	14 (7%)	6 (3%)	5 13
1	E	201/209 (96%)	186 (92%)	13 (6%)	2 (1%)	19 45
1	F	197/209 (94%)	183 (93%)	13 (7%)	1 (0%)	34 63
All	All	1185/1254 (94%)	1110 (94%)	62 (5%)	13 (1%)	17 42

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	642	SER
1	F	582	LYS
1	A	694	ALA
1	D	526	GLY
1	D	543	GLU
1	A	641	LEU
1	C	498	ASP
1	C	523	GLU
1	E	643	SER

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Mol	Chain	Res	Type
1	D	532	LYS
1	D	581	GLY
1	D	528	VAL
1	D	529	PRO

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	162/171 (95%)	156 (96%)	6 (4%)	41 72
1	B	162/171 (95%)	157 (97%)	5 (3%)	47 78
1	C	162/171 (95%)	155 (96%)	7 (4%)	35 66
1	D	162/171 (95%)	158 (98%)	4 (2%)	55 84
1	E	165/171 (96%)	162 (98%)	3 (2%)	66 89
1	F	162/171 (95%)	158 (98%)	4 (2%)	55 84
All	All	975/1026 (95%)	946 (97%)	29 (3%)	48 79

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	ASP
1	A	599	ARG
1	A	615	ASN
1	A	623	LYS
1	A	637	ARG
1	A	678	GLN
1	B	518	GLN
1	B	587	ILE
1	B	591	SER
1	B	615	ASN
1	B	658	VAL
1	C	538	ARG
1	C	544	VAL
1	C	587	ILE

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Mol	Chain	Res	Type
1	C	599	ARG
1	C	615	ASN
1	C	623	LYS
1	C	678	GLN
1	D	519	PHE
1	D	531	LEU
1	D	553	LYS
1	D	615	ASN
1	E	582	LYS
1	E	587	ILE
1	E	615	ASN
1	F	580	ASN
1	F	615	ASN
1	F	642	SER
1	F	672	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	507	GLN
1	A	615	ASN
1	A	620	ASN
1	A	678	GLN
1	B	507	GLN
1	B	615	ASN
1	B	620	ASN
1	B	624	GLN
1	B	678	GLN
1	B	686	HIS
1	C	507	GLN
1	C	615	ASN
1	C	620	ASN
1	C	633	HIS
1	C	678	GLN
1	D	507	GLN
1	D	615	ASN
1	D	620	ASN
1	D	624	GLN
1	D	678	GLN
1	D	686	HIS
1	E	496	GLN
1	E	615	ASN

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Mol	Chain	Res	Type
1	E	620	ASN
1	E	678	GLN
1	E	686	HIS
1	F	518	GLN
1	F	580	ASN
1	F	615	ASN
1	F	620	ASN
1	F	624	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

11 ligands are 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	$\#\|Z\| > 2$
2	SO4	A	1696	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	1697	-	4,4,4	0.22	0	6,6,6	0.13	0
2	SO4	C	1696	-	4,4,4	0.22	0	6,6,6	0.13	0
2	SO4	C	1697	-	4,4,4	0.21	0	6,6,6	0.08	0
2	SO4	D	1696	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	E	1695	-	4,4,4	0.22	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	F	1696	-	4,4,4	0.19	0	6,6,6	0.17	0
2	SO4	F	1697	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	F	1698	-	4,4,4	0.27	0	6,6,6	0.10	0
2	SO4	F	1699	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	F	1700	-	4,4,4	1.18	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1696	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1697	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1696	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1697	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1696	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1695	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1696	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1697	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1698	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1699	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1700	-	-	0/0/0/0	0/0/0/0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1697	SO4	1	0
2	C	1696	SO4	1	0

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	199/209 (95%)	-0.10	3 (1%) 76 76	23, 35, 53, 63	0
1	B	198/209 (94%)	-0.05	7 (3%) 48 48	21, 36, 55, 66	0
1	C	199/209 (95%)	0.01	12 (6%) 25 24	22, 36, 67, 84	0
1	D	199/209 (95%)	0.24	18 (9%) 12 9	20, 37, 82, 100	0
1	E	203/209 (97%)	0.04	9 (4%) 38 37	23, 40, 65, 81	0
1	F	199/209 (95%)	0.30	15 (7%) 17 15	21, 38, 83, 94	0
All	All	1197/1254 (95%)	0.08	64 (5%) 30 28	20, 37, 70, 100	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	497	ALA	9.5
1	F	526	GLY	8.6
1	B	497	ALA	7.8
1	A	497	ALA	6.4
1	D	497	ALA	5.6
1	D	526	GLY	5.2
1	D	544	VAL	5.2
1	D	522	PRO	5.0
1	C	497	ALA	4.9
1	F	583	GLY	4.3
1	F	523	GLU	4.3
1	E	524	ALA	4.3
1	E	523	GLU	4.1
1	C	526	GLY	4.1
1	D	644	GLU	4.1
1	D	524	ALA	4.0
1	D	581	GLY	4.0
1	E	612	GLU	3.8
1	D	528	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	695	HIS	3.6
1	E	525	THR	3.6
1	F	524	ALA	3.6
1	D	498	ASP	3.6
1	D	527	GLY	3.5
1	A	612	GLU	3.4
1	F	528	VAL	3.3
1	F	525	THR	3.3
1	E	527	GLY	3.2
1	E	557	MET	3.2
1	C	557	MET	3.2
1	F	553	LYS	3.1
1	C	523	GLU	3.1
1	B	693	ALA	3.1
1	D	523	GLU	3.1
1	F	582	LYS	3.0
1	E	644	GLU	3.0
1	B	612	GLU	3.0
1	C	498	ASP	3.0
1	D	612	GLU	3.0
1	E	662	SER	2.9
1	C	695	HIS	2.9
1	F	695	HIS	2.8
1	D	531	LEU	2.8
1	C	528	VAL	2.8
1	C	644	GLU	2.8
1	D	525	THR	2.7
1	F	529	PRO	2.7
1	E	661	LYS	2.7
1	F	498	ASP	2.6
1	D	583	GLY	2.6
1	C	524	ALA	2.5
1	C	672	TYR	2.5
1	B	544	VAL	2.5
1	D	521	GLU	2.5
1	D	529	PRO	2.4
1	B	661	LYS	2.4
1	F	557	MET	2.3
1	A	647	PRO	2.2
1	B	644	GLU	2.2
1	C	694	ALA	2.2
1	F	694	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	556	SER	2.1
1	B	613	ASP	2.0
1	C	529	PRO	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	F	1699	5/5	0.90	0.20	1.30	91,91,91,91	0
2	SO4	F	1698	5/5	0.89	0.18	1.11	91,92,93,93	0
2	SO4	A	1697	5/5	0.94	0.25	0.70	83,84,84,84	0
2	SO4	F	1697	5/5	0.95	0.28	0.43	79,79,79,79	0
2	SO4	A	1696	5/5	0.95	0.15	0.22	68,69,69,69	0
2	SO4	C	1696	5/5	0.99	0.12	-0.75	37,38,40,41	0
2	SO4	F	1696	5/5	0.98	0.09	-1.37	37,38,39,39	0
2	SO4	C	1697	5/5	0.97	0.11	-2.41	76,76,77,77	0
2	SO4	F	1700	5/5	0.85	0.30	-	78,78,80,80	0
2	SO4	E	1695	5/5	0.94	0.24	-	87,88,88,88	0
2	SO4	D	1696	5/5	0.94	0.35	-	96,97,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.