Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:27 PM GMT

PDB ID	:	1FI1
Title	:	FhuA in complex with lipopolysaccharide and rifamycin CGP4832
Authors	:	Ferguson, A.D.; Koedding, J.; Boes, C.; Walker, G.; Coulton, J.W.; Diederichs, K.; Braun, V.; Welte, W.
Deposited on	:	2000-08-03
Resolution	:	2.90 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:

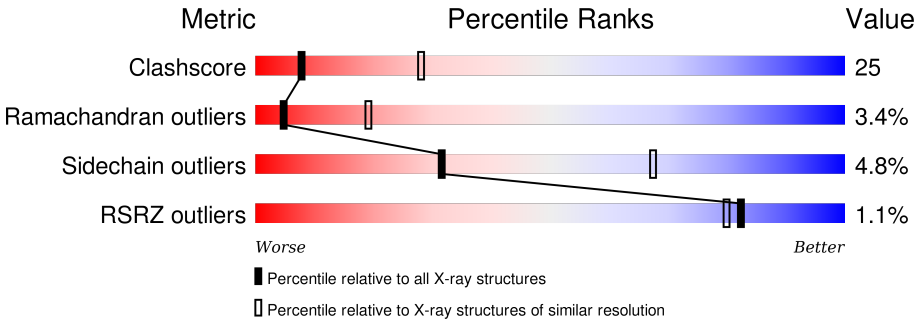
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	707	% 56% 39% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	DDQ	A	1023	-	-	-	X
2	GCN	A	1001	X	-	-	-
2	FTT	A	1004	-	-	-	X
2	GMH	A	1011	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GMH	A	1012	X	-	-	-
5	NA	A	1024	-	-	-	X
7	FTT	A	1002	X	-	-	X
7	FTT	A	1006	X	-	-	-
7	FTT	A	1007	-	-	-	X
9	RIF	A	1022	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6030 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 FERRICHROME-IRON RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	707	Total	C	N	O	S	0	0	0
			5523	3475	944	1090	14			

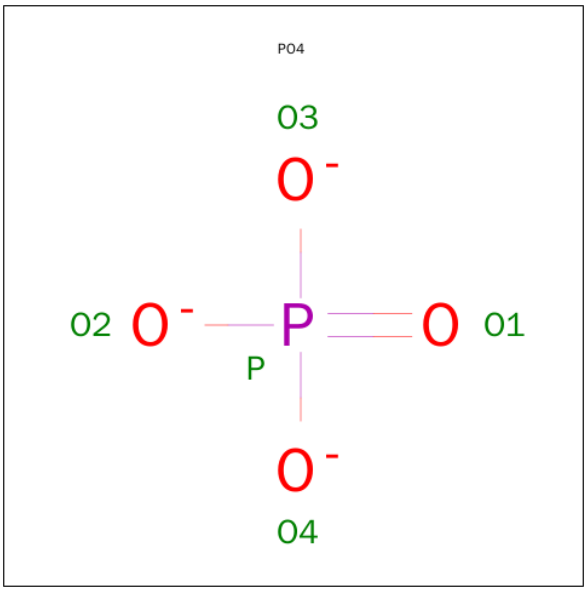
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	INTRACHAIN HIS TAG	UNP P06971
A	407	SER	-	INTRACHAIN HIS TAG	UNP P06971
A	408	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	409	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	410	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	411	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	412	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	413	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	414	GLY	-	INTRACHAIN HIS TAG	UNP P06971
A	415	SER	-	INTRACHAIN HIS TAG	UNP P06971
A	416	SER	-	INTRACHAIN HIS TAG	UNP P06971

- Molecule 2 is a polymer of unknown type called SUGAR (12-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	12	Total	C	N	O	0	0
			150	87	2	61		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 4 3 1	0	0
3	A	1	Total O P 4 3 1	0	0

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ni 1 1	0	0

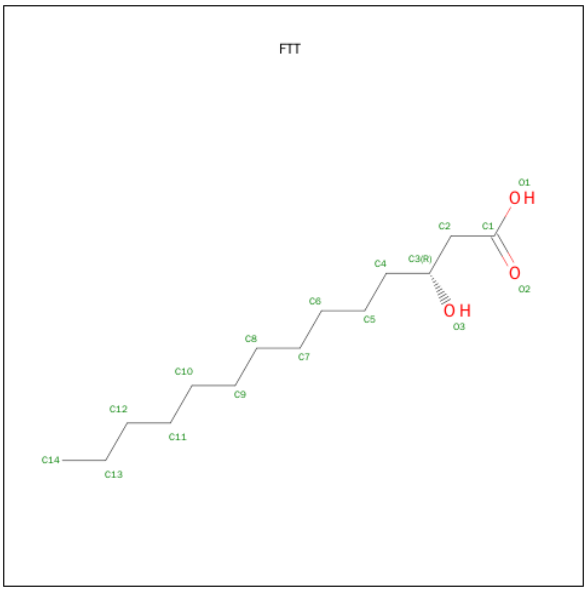
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

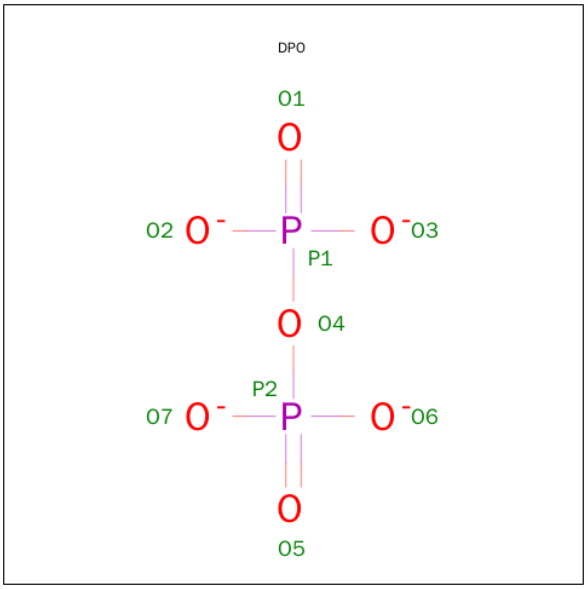
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0

- Molecule 7 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula: $C_{14}H_{28}O_3$).



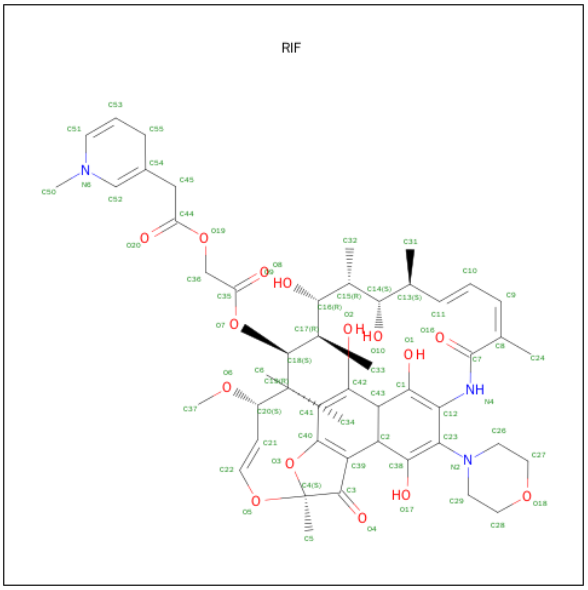
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 16 14 2	0	0
7	A	1	Total C O 9 6 3	0	0
7	A	1	Total C O 13 12 1	0	0
7	A	1	Total C O 17 14 3	0	0
7	A	1	Total C O 15 14 1	0	0

- Molecule 8 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2).



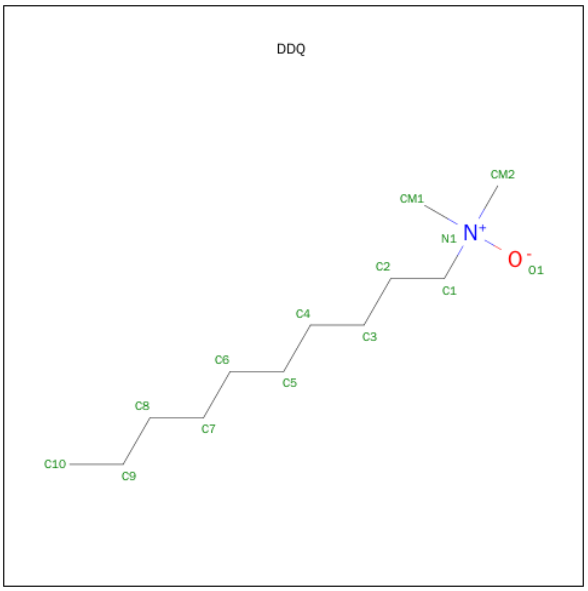
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O P 8 6 2	0	0
8	A	1	Total O P 8 6 2	0	0

- Molecule 9 is RIFAMYCIN CGP 4832 (three-letter code: RIF) (formula: $C_{49}H_{65}N_3O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 67 49 3 15	0	0

- Molecule 10 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: $C_{12}H_{27}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	12	1	1		

- Molecule 11 is water.

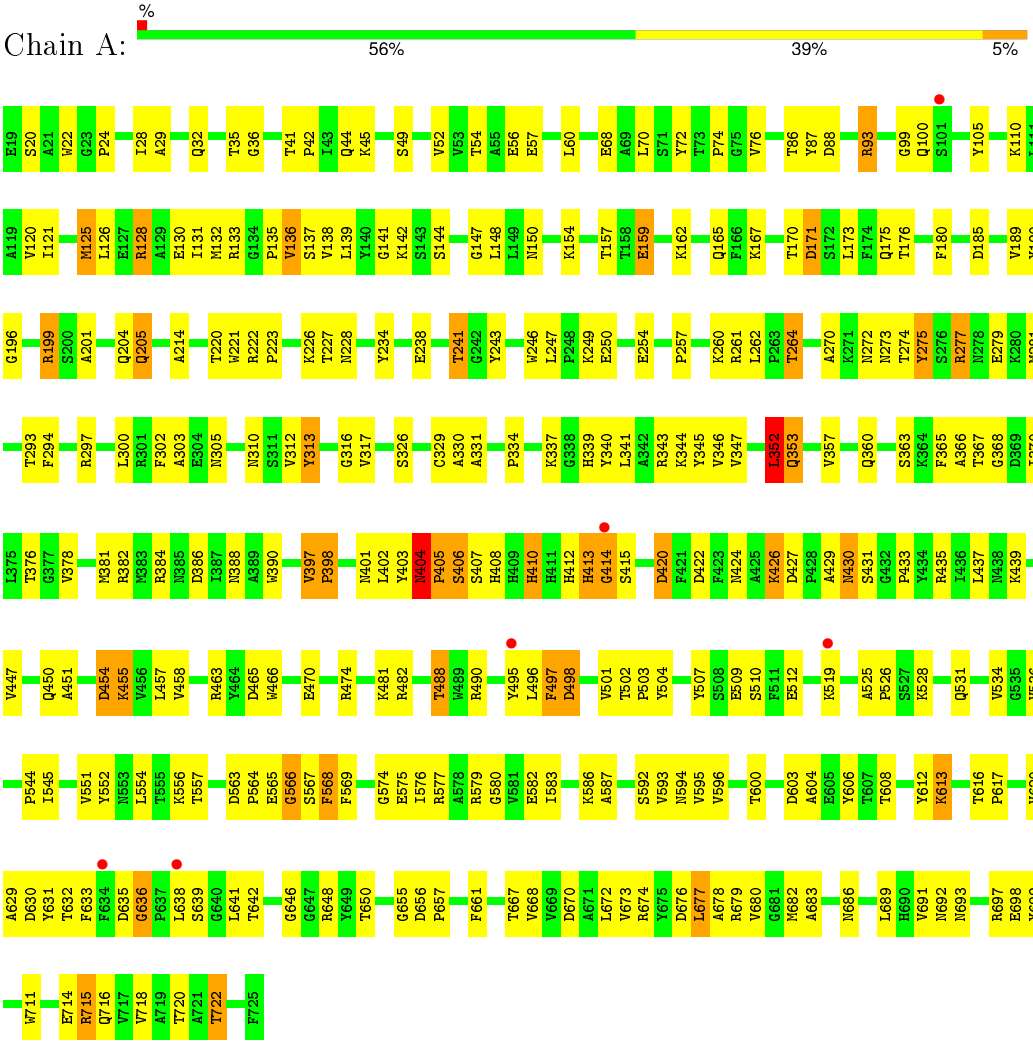
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	179	Total	O	0	0
			179	179		

3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	172.82Å 172.82Å 87.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.90 41.51 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.90) 97.9 (41.51-2.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.71 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.275 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	62.1	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 65.2	EDS
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 33363 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6030	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: NI, MG, GMH, FTT, PA1, GLA, PO4, GLC, GCN, DPO, KDO, NA, RIF, DDQ

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	0.39	0/5663	0.65	1/7696 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	5	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	352	LEU	CA-CB-CG	5.04	126.89	115.30

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	GCN	C1
2	A	1011	GMH	C6,C1
2	A	1012	GMH	C6,C1

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	5523	0	5223	273	0
2	A	150	0	129	2	0
3	A	8	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	70	0	104	15	0
8	A	16	0	0	1	0
9	A	67	0	61	4	0
10	A	14	0	27	0	0
11	A	179	0	0	8	0
All	All	6030	0	5544	285	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 25.

All (285) 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:274:THR:HG22	1:A:310:ASN:HB2	1.41	1.00
1:A:277:ARG:HH11	1:A:277:ARG:HG2	1.34	0.91
1:A:70:LEU:HD13	1:A:131:ILE:HD11	1.51	0.91
1:A:624:MET:HA	11:A:1179:HOH:O	1.71	0.89
1:A:74:PRO:HG2	1:A:133:ARG:HH12	1.37	0.88
1:A:404:ASN:H	1:A:405:PRO:HD3	1.37	0.88
1:A:404:ASN:N	1:A:405:PRO:HD3	1.90	0.87
1:A:382:ARG:HD2	7:A:1002:FTT:H21	1.56	0.86
7:A:1002:FTT:O2	7:A:1002:FTT:H42	1.77	0.85
1:A:262:LEU:HD21	1:A:402:LEU:HG	1.57	0.84
1:A:545:ILE:HG22	1:A:587:ALA:HB1	1.60	0.83
1:A:52:VAL:HG22	1:A:130:GLU:HG2	1.61	0.82
1:A:238:GLU:OE1	1:A:277:ARG:NH1	2.12	0.82
1:A:650:THR:HA	11:A:1179:HOH:O	1.80	0.81
1:A:136:VAL:HG21	1:A:148:LEU:HD22	1.60	0.81
1:A:277:ARG:HH11	1:A:277:ARG:CG	1.96	0.79
1:A:382:ARG:CD	7:A:1002:FTT:H21	2.13	0.78
1:A:401:ASN:OD1	1:A:403:TYR:HB2	1.84	0.77
1:A:70:LEU:HD13	1:A:131:ILE:CD1	2.15	0.76
1:A:44:GLN:HE21	1:A:45:LYS:HG3	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1002:FTT:H101	7:A:1005:FTT:H62	1.68	0.75
1:A:170:THR:HG22	1:A:171:ASP:H	1.50	0.75
1:A:74:PRO:HG2	1:A:133:ARG:NH1	2.01	0.74
1:A:612:TYR:O	1:A:613:LYS:HB2	1.88	0.74
1:A:496:LEU:HA	1:A:502:THR:HG23	1.70	0.73
7:A:1002:FTT:O2	7:A:1002:FTT:C4	2.33	0.73
1:A:586:LYS:HG2	1:A:596:VAL:HG22	1.69	0.73
1:A:470:GLU:HG3	1:A:481:LYS:HG2	1.71	0.73
1:A:397:VAL:HG23	1:A:398:PRO:HD2	1.69	0.73
1:A:639:SER:HB3	1:A:679:ARG:NH1	2.04	0.72
1:A:628:TRP:CH2	1:A:630:ASP:HB3	2.23	0.72
1:A:162:LYS:HA	1:A:180:PHE:HD1	1.55	0.72
1:A:226:LYS:HB3	1:A:289:GLU:HB3	1.72	0.72
1:A:167:LYS:HB2	1:A:175:GLN:HB3	1.72	0.71
1:A:430:ASN:HD22	1:A:431:SER:N	1.87	0.71
1:A:692:ASN:O	1:A:715:ARG:HA	1.90	0.71
2:A:1010:GMH:H6	8:A:1015:DPO:O6	1.91	0.71
1:A:474:ARG:HH11	1:A:474:ARG:HG2	1.56	0.70
1:A:159:GLU:H	1:A:159:GLU:CD	1.95	0.70
1:A:162:LYS:HA	1:A:180:PHE:CD1	2.27	0.70
1:A:205:GLN:HG3	1:A:243:TYR:CG	2.27	0.70
1:A:112:GLN:HG3	1:A:381:MET:HE1	1.74	0.70
1:A:35:THR:HG22	1:A:150:ASN:HD22	1.54	0.69
1:A:352:LEU:HB2	1:A:384:ARG:O	1.93	0.69
1:A:189:VAL:HG13	1:A:190:TYR:CD2	2.28	0.68
1:A:404:ASN:N	1:A:405:PRO:CD	2.57	0.68
1:A:600:THR:HB	1:A:624:MET:HB2	1.76	0.67
1:A:135:PRO:HB3	1:A:510:SER:HB3	1.75	0.67
1:A:648:ARG:NH1	1:A:670:ASP:OD2	2.27	0.67
1:A:36:GLY:HA2	1:A:132:MET:CE	2.25	0.66
1:A:112:GLN:HG3	1:A:381:MET:CE	2.26	0.66
1:A:300:LEU:HD12	1:A:357:VAL:CG1	2.26	0.66
1:A:264:THR:HA	1:A:711:TRP:CD1	2.32	0.64
1:A:35:THR:CG2	1:A:150:ASN:HD22	2.11	0.64
1:A:99:GLY:O	1:A:100:GLN:HB2	1.97	0.64
1:A:343:ARG:O	1:A:397:VAL:HG13	1.98	0.64
1:A:592:SER:HB2	1:A:632:THR:O	1.97	0.64
1:A:125:MET:HG3	1:A:234:TYR:HE1	1.63	0.63
1:A:88:ASP:OD2	1:A:120:VAL:HG22	1.98	0.63
1:A:302:PHE:CZ	7:A:1006:FTT:H22	2.34	0.62
1:A:42:PRO:HB2	1:A:44:GLN:HE22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.64	0.62
1:A:454:ASP:O	1:A:455:LYS:HB2	1.98	0.62
1:A:412:HIS:O	1:A:414:GLY:N	2.32	0.62
1:A:592:SER:O	1:A:631:TYR:HA	1.99	0.62
1:A:24:PRO:O	1:A:28:ILE:HG12	2.00	0.62
1:A:406:SER:C	1:A:408:HIS:H	2.03	0.61
1:A:670:ASP:OD1	1:A:692:ASN:HA	2.01	0.61
1:A:455:LYS:HE2	1:A:455:LYS:N	2.15	0.61
1:A:704:PHE:CE2	1:A:708:GLY:HA3	2.36	0.61
9:A:1022:RIF:O4	9:A:1022:RIF:H501	1.99	0.61
1:A:170:THR:HG22	1:A:171:ASP:N	2.15	0.59
1:A:430:ASN:HD22	1:A:430:ASN:C	2.05	0.59
1:A:715:ARG:HH11	1:A:715:ARG:HG2	1.66	0.59
1:A:633:PHE:HB2	1:A:638:LEU:O	2.02	0.59
1:A:93:ARG:HG3	1:A:552:TYR:OH	2.01	0.59
7:A:1002:FTT:C10	7:A:1005:FTT:H62	2.32	0.59
1:A:567:SER:O	1:A:568:PHE:HB2	2.02	0.59
1:A:56:GLU:H	1:A:56:GLU:CD	2.06	0.59
7:A:1006:FTT:H143	7:A:1007:FTT:H92	1.84	0.59
1:A:167:LYS:HG3	1:A:720:THR:HG23	1.85	0.58
1:A:249:LYS:HG2	1:A:250:GLU:OE1	2.03	0.58
1:A:397:VAL:O	1:A:398:PRO:O	2.21	0.58
1:A:577:ARG:CZ	1:A:579:ARG:HE	2.15	0.58
1:A:612:TYR:O	1:A:613:LYS:CB	2.50	0.58
1:A:413:HIS:O	1:A:415:SER:N	2.37	0.57
1:A:42:PRO:HG2	1:A:45:LYS:HG3	1.86	0.57
1:A:366:ALA:HB2	1:A:371:ASP:HA	1.86	0.57
1:A:264:THR:HG21	1:A:698:GLU:HG2	1.86	0.57
1:A:592:SER:HG	1:A:631:TYR:HE1	1.53	0.57
1:A:404:ASN:H	1:A:405:PRO:CD	2.15	0.57
1:A:594:ASN:HB2	1:A:630:ASP:OD1	2.05	0.57
1:A:196:GLY:HA2	1:A:214:ALA:O	2.05	0.57
1:A:668:VAL:HG13	1:A:693:ASN:HA	1.87	0.56
1:A:531:GLN:HB2	1:A:554:LEU:HD13	1.86	0.56
1:A:93:ARG:HD2	1:A:582:GLU:OE2	2.05	0.56
1:A:221:TRP:CE2	1:A:223:PRO:HG3	2.39	0.56
1:A:249:LYS:HE2	1:A:254:GLU:OE1	2.04	0.56
1:A:86:THR:O	1:A:277:ARG:NH2	2.39	0.56
1:A:316:GLY:O	1:A:341:LEU:HD12	2.06	0.56
1:A:604:ALA:O	1:A:616:THR:HG22	2.04	0.56
1:A:246:TRP:O	1:A:247:LEU:HD23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ASN:HD22	1:A:435:ARG:HG2	1.70	0.56
1:A:667:THR:H	1:A:697:ARG:NH1	2.04	0.56
1:A:642:THR:HB	1:A:674:ARG:HB3	1.88	0.55
1:A:74:PRO:HB2	1:A:582:GLU:HB3	1.88	0.55
1:A:273:ASN:HD21	1:A:312:VAL:H	1.54	0.55
1:A:313:TYR:OH	9:A:1022:RIF:H243	2.08	0.54
1:A:457:LEU:HD12	1:A:458:VAL:N	2.23	0.54
1:A:563:ASP:OD1	1:A:564:PRO:HD2	2.08	0.54
1:A:474:ARG:HG2	1:A:474:ARG:NH1	2.23	0.53
1:A:303:ALA:O	1:A:353:GLN:HA	2.09	0.53
1:A:390:TRP:CE2	1:A:426:LYS:HB2	2.44	0.53
1:A:446:TYR:HB3	1:A:463:ARG:HB2	1.89	0.53
1:A:488:THR:HG22	1:A:509:GLU:HB2	1.91	0.53
1:A:49:SER:HB3	11:A:1128:HOH:O	2.09	0.53
1:A:366:ALA:CB	1:A:371:ASP:HA	2.39	0.53
1:A:144:SER:HA	1:A:512:GLU:OE1	2.09	0.53
1:A:300:LEU:HB2	1:A:357:VAL:HG12	1.91	0.53
1:A:300:LEU:HD12	1:A:357:VAL:HG12	1.90	0.53
1:A:378:VAL:HG12	1:A:445:VAL:HG12	1.89	0.53
1:A:192:TYR:C	1:A:192:TYR:CD1	2.82	0.53
1:A:189:VAL:HG23	1:A:222:ARG:O	2.09	0.52
1:A:121:ILE:HG21	1:A:126:LEU:HD21	1.91	0.52
1:A:384:ARG:NH2	2:A:1009:KDO:O1B	2.41	0.52
1:A:344:LYS:HD3	9:A:1022:RIF:H242	1.91	0.52
1:A:451:ALA:O	1:A:458:VAL:HG12	2.10	0.52
1:A:36:GLY:HA2	1:A:132:MET:HE3	1.91	0.52
1:A:390:TRP:CE2	1:A:426:LYS:HG3	2.44	0.52
1:A:574:GLY:HA2	1:A:608:THR:O	2.09	0.52
1:A:376:THR:HG22	1:A:447:VAL:HG22	1.92	0.52
1:A:678:ALA:CB	1:A:683:ALA:HA	2.41	0.51
1:A:138:VAL:HG13	1:A:139:LEU:HG	1.93	0.51
1:A:677:LEU:HB2	1:A:686:ASN:HA	1.93	0.51
1:A:45:LYS:HB3	1:A:457:LEU:CD2	2.40	0.51
1:A:44:GLN:NE2	1:A:45:LYS:HG3	2.23	0.51
1:A:655:GLY:O	1:A:656:ASP:HB3	2.11	0.51
1:A:241:THR:HB	1:A:275:TYR:HB3	1.93	0.51
1:A:257:PRO:HD2	1:A:339:HIS:HB3	1.93	0.51
7:A:1006:FTT:H122	7:A:1007:FTT:C9	2.41	0.51
1:A:370:ILE:HG22	1:A:372:HIS:NE2	2.25	0.51
1:A:595:VAL:HG12	1:A:629:ALA:HB2	1.93	0.50
1:A:173:LEU:HA	1:A:201:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:THR:HG22	1:A:575:GLU:HG3	1.92	0.50
1:A:576:ILE:HD11	1:A:606:TYR:CE1	2.47	0.50
1:A:384:ARG:NH1	1:A:439:LYS:HE2	2.27	0.50
1:A:595:VAL:HG12	1:A:629:ALA:CB	2.42	0.50
1:A:56:GLU:N	1:A:56:GLU:CD	2.65	0.49
1:A:386:ASP:OD2	1:A:437:LEU:HD13	2.12	0.49
1:A:326:SER:HB3	1:A:329:CYS:HB2	1.94	0.49
1:A:157:THR:HB	1:A:159:GLU:OE2	2.12	0.49
1:A:185:ASP:CG	1:A:189:VAL:HG12	2.33	0.49
1:A:199:ARG:HG3	1:A:199:ARG:NH1	2.27	0.49
1:A:373:THR:HB	1:A:450:GLN:HB2	1.95	0.49
1:A:167:LYS:CG	1:A:720:THR:HG23	2.42	0.48
1:A:72:TYR:CE2	1:A:628:TRP:HB2	2.48	0.48
1:A:60:LEU:HD21	1:A:628:TRP:HH2	1.78	0.48
1:A:676:ASP:C	1:A:678:ALA:H	2.16	0.48
1:A:363:SER:HB2	1:A:374:LEU:HB3	1.95	0.48
1:A:32:GLN:O	1:A:128:ARG:NH2	2.43	0.48
1:A:633:PHE:CE2	1:A:641:LEU:HD23	2.48	0.48
1:A:261:ARG:O	1:A:405:PRO:HB3	2.13	0.48
1:A:192:TYR:HD1	1:A:193:ARG:N	2.11	0.48
1:A:390:TRP:CZ3	1:A:433:PRO:HB3	2.48	0.48
1:A:501:VAL:HG23	1:A:501:VAL:O	2.13	0.48
1:A:406:SER:C	1:A:408:HIS:N	2.68	0.47
1:A:330:ALA:HA	1:A:337:LYS:NZ	2.29	0.47
1:A:612:TYR:CZ	1:A:657:PRO:HB2	2.50	0.47
1:A:154:LYS:HD3	1:A:193:ARG:NH2	2.29	0.47
1:A:579:ARG:O	1:A:603:ASP:HB3	2.14	0.47
1:A:672:LEU:HD12	1:A:672:LEU:C	2.35	0.47
1:A:288:HIS:HD2	1:A:289:GLU:N	2.13	0.47
1:A:317:VAL:HA	1:A:340:TYR:O	2.15	0.47
1:A:275:TYR:OH	11:A:1102:HOH:O	2.08	0.47
1:A:495:TYR:O	1:A:503:PRO:HD2	2.15	0.47
1:A:593:VAL:HG23	1:A:631:TYR:CD1	2.50	0.46
1:A:503:PRO:HA	1:A:536:VAL:HG12	1.97	0.46
7:A:1006:FTT:H143	7:A:1007:FTT:H112	1.97	0.46
7:A:1006:FTT:C7	7:A:1007:FTT:H41	2.45	0.46
1:A:297:ARG:HG3	1:A:360:GLN:HG3	1.97	0.46
1:A:592:SER:CB	1:A:632:THR:O	2.61	0.46
1:A:367:THR:HB	1:A:370:ILE:HB	1.95	0.46
1:A:165:GLN:HG3	1:A:722:THR:HB	1.97	0.46
1:A:370:ILE:HG22	1:A:372:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:TYR:CE2	1:A:537:LYS:HG3	2.51	0.46
1:A:42:PRO:CB	1:A:44:GLN:HE22	2.28	0.46
1:A:302:PHE:HZ	7:A:1006:FTT:H22	1.81	0.46
1:A:673:VAL:HG23	1:A:673:VAL:O	2.16	0.46
1:A:185:ASP:OD2	1:A:189:VAL:HG12	2.16	0.46
1:A:567:SER:O	1:A:568:PHE:CB	2.64	0.46
1:A:93:ARG:HG3	1:A:552:TYR:CZ	2.50	0.46
1:A:228:ASN:HB3	1:A:287:ASP:OD1	2.16	0.46
1:A:344:LYS:HD3	9:A:1022:RIF:C24	2.46	0.46
1:A:365:PHE:HD1	1:A:366:ALA:N	2.13	0.45
1:A:281:MET:HB3	1:A:303:ALA:HB2	1.97	0.45
1:A:68:GLU:CD	1:A:68:GLU:H	2.20	0.45
1:A:628:TRP:HD1	1:A:646:GLY:HA3	1.81	0.45
1:A:390:TRP:NE1	1:A:426:LYS:HB2	2.31	0.45
1:A:504:TYR:HE2	1:A:537:LYS:HG3	1.82	0.45
1:A:583:ILE:HG13	1:A:583:ILE:O	2.14	0.45
1:A:279:GLU:HA	1:A:305:ASN:OD1	2.17	0.45
1:A:397:VAL:HG23	1:A:398:PRO:CD	2.42	0.45
1:A:273:ASN:ND2	1:A:312:VAL:H	2.15	0.45
1:A:680:VAL:HG12	1:A:680:VAL:O	2.17	0.45
1:A:628:TRP:CZ3	1:A:630:ASP:OD1	2.69	0.45
1:A:427:ASP:OD1	1:A:429:ALA:HB3	2.17	0.45
1:A:142:LYS:HG2	1:A:442:GLN:OE1	2.17	0.45
1:A:93:ARG:HH11	1:A:582:GLU:CD	2.20	0.45
1:A:260:LYS:HB2	1:A:405:PRO:HG2	1.98	0.45
1:A:457:LEU:HD12	1:A:458:VAL:H	1.81	0.45
1:A:204:GLN:OE1	1:A:714:GLU:HG2	2.16	0.45
1:A:300:LEU:C	1:A:300:LEU:HD23	2.37	0.44
1:A:70:LEU:HD13	1:A:131:ILE:CG1	2.48	0.44
1:A:715:ARG:NH1	1:A:715:ARG:HG2	2.29	0.44
1:A:110:LYS:HD3	1:A:112:GLN:HG2	1.99	0.44
1:A:676:ASP:O	1:A:678:ALA:N	2.49	0.44
1:A:345:TYR:CD1	1:A:345:TYR:C	2.90	0.44
1:A:70:LEU:CD1	1:A:131:ILE:HD11	2.36	0.44
1:A:192:TYR:CD1	1:A:193:ARG:N	2.86	0.44
1:A:317:VAL:HG22	11:A:1176:HOH:O	2.18	0.44
1:A:41:THR:CG2	1:A:45:LYS:HB2	2.47	0.44
1:A:137:SER:OG	1:A:510:SER:HA	2.18	0.44
1:A:223:PRO:HD2	1:A:227:THR:HG22	2.01	0.43
1:A:270:ALA:HB1	1:A:272:ASN:OD1	2.18	0.43
1:A:545:ILE:HG22	1:A:587:ALA:CB	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LEU:CA	1:A:502:THR:HG23	2.44	0.43
7:A:1006:FTT:H3	7:A:1007:FTT:H22	1.34	0.43
1:A:221:TRP:CZ2	1:A:223:PRO:HG3	2.53	0.43
1:A:87:TYR:OH	11:A:1102:HOH:O	2.20	0.43
1:A:482:ARG:NH2	1:A:526:PRO:HD3	2.33	0.43
1:A:105:TYR:CE2	1:A:110:LYS:HB2	2.53	0.43
1:A:341:LEU:HB2	1:A:402:LEU:CD1	2.48	0.43
1:A:36:GLY:HA2	1:A:132:MET:HE1	1.97	0.43
1:A:24:PRO:HB3	1:A:544:PRO:HB3	2.00	0.43
1:A:370:ILE:HG22	1:A:370:ILE:O	2.18	0.43
1:A:635:ASP:O	1:A:636:GLY:O	2.37	0.43
1:A:165:GLN:HE21	1:A:722:THR:HB	1.82	0.43
1:A:565:GLU:O	1:A:566:GLY:C	2.57	0.43
1:A:714:GLU:O	1:A:715:ARG:C	2.57	0.43
1:A:176:THR:HG23	1:A:176:THR:O	2.19	0.42
1:A:699:TYR:N	1:A:699:TYR:CD1	2.87	0.42
1:A:22:TRP:CD2	1:A:60:LEU:HD22	2.55	0.42
1:A:538:TYR:CE2	1:A:540:PRO:HG3	2.55	0.42
1:A:148:LEU:HD23	1:A:148:LEU:N	2.34	0.42
1:A:412:HIS:O	1:A:413:HIS:C	2.56	0.42
1:A:28:ILE:HG13	1:A:29:ALA:N	2.35	0.42
1:A:294:PHE:HE1	1:A:363:SER:OG	2.01	0.42
1:A:519:LYS:HA	1:A:569:PHE:CD2	2.54	0.42
1:A:422:ASP:OD1	1:A:424:ASN:N	2.52	0.42
1:A:692:ASN:O	1:A:693:ASN:HB3	2.19	0.42
1:A:132:MET:O	1:A:147:GLY:CA	2.67	0.42
1:A:673:VAL:CG2	1:A:689:LEU:HB3	2.49	0.42
1:A:382:ARG:HD2	7:A:1002:FTT:C2	2.40	0.42
1:A:220:THR:HG22	1:A:221:TRP:N	2.33	0.42
1:A:288:HIS:CD2	1:A:289:GLU:N	2.87	0.42
1:A:99:GLY:O	1:A:100:GLN:CB	2.67	0.42
1:A:678:ALA:HA	1:A:682:MET:O	2.19	0.42
1:A:93:ARG:HA	11:A:1115:HOH:O	2.19	0.42
1:A:381:MET:HG2	11:A:1086:HOH:O	2.19	0.42
1:A:528:LYS:O	1:A:556:LYS:HA	2.19	0.42
1:A:22:TRP:CE2	1:A:60:LEU:HD22	2.54	0.41
1:A:112:GLN:HG3	1:A:381:MET:HE3	2.01	0.41
1:A:631:TYR:CE2	1:A:633:PHE:CE1	3.08	0.41
1:A:264:THR:CG2	1:A:698:GLU:HG2	2.50	0.41
1:A:403:TYR:O	1:A:404:ASN:ND2	2.53	0.41
1:A:44:GLN:HB3	1:A:539:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PHE:O	1:A:193:ARG:HA	2.19	0.41
1:A:617:PRO:O	1:A:620:VAL:HG12	2.20	0.41
1:A:346:VAL:HG22	1:A:347:VAL:N	2.36	0.41
1:A:633:PHE:CD2	1:A:641:LEU:HD23	2.56	0.41
1:A:173:LEU:HD23	1:A:718:VAL:HG22	2.02	0.41
1:A:442:GLN:HA	1:A:466:TRP:O	2.20	0.41
1:A:54:THR:HG23	1:A:57:GLU:OE2	2.21	0.41
1:A:427:ASP:HB3	1:A:430:ASN:ND2	2.36	0.41
1:A:205:GLN:HG3	1:A:243:TYR:CB	2.51	0.41
1:A:141:GLY:HA2	1:A:465:ASP:OD2	2.21	0.41
1:A:490:ARG:HG3	1:A:507:TYR:O	2.20	0.41
1:A:310:ASN:ND2	1:A:347:VAL:HG22	2.37	0.40
1:A:497:PHE:HB3	1:A:498:ASP:H	1.63	0.40
1:A:105:TYR:O	1:A:150:ASN:HA	2.22	0.40
1:A:482:ARG:CZ	1:A:525:ALA:HA	2.51	0.40
1:A:691:VAL:HA	1:A:716:GLN:O	2.21	0.40
1:A:551:VAL:HA	1:A:580:GLY:O	2.21	0.40
7:A:1002:FTT:H112	7:A:1002:FTT:H142	1.89	0.40
1:A:42:PRO:HG2	1:A:45:LYS:CG	2.51	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	705/707 (100%)	621 (88%)	60 (8%)	24 (3%)	5 19

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	PRO
1	A	406	SER

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Mol	Chain	Res	Type
1	A	413	HIS
1	A	613	LYS
1	A	20	SER
1	A	368	GLY
1	A	405	PRO
1	A	410	HIS
1	A	414	GLY
1	A	497	PHE
1	A	498	ASP
1	A	566	GLY
1	A	636	GLY
1	A	677	LEU
1	A	264	THR
1	A	171	ASP
1	A	407	SER
1	A	420	ASP
1	A	454	ASP
1	A	715	ARG
1	A	331	ALA
1	A	334	PRO
1	A	404	ASN
1	A	136	VAL

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	587/587 (100%)	559 (95%)	28 (5%)	31 67

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	VAL
1	A	93	ARG
1	A	112	GLN
1	A	118	ASP

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Mol	Chain	Res	Type
1	A	125	MET
1	A	128	ARG
1	A	159	GLU
1	A	199	ARG
1	A	205	GLN
1	A	241	THR
1	A	275	TYR
1	A	277	ARG
1	A	293	THR
1	A	313	TYR
1	A	352	LEU
1	A	353	GLN
1	A	397	VAL
1	A	404	ASN
1	A	410	HIS
1	A	420	ASP
1	A	426	LYS
1	A	430	ASN
1	A	455	LYS
1	A	488	THR
1	A	534	VAL
1	A	568	PHE
1	A	661	PHE
1	A	722	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	44	GLN
1	A	112	GLN
1	A	150	ASN
1	A	165	GLN
1	A	202	ASN
1	A	288	HIS
1	A	310	ASN
1	A	328	GLN
1	A	339	HIS
1	A	354	ASN
1	A	388	ASN
1	A	404	ASN
1	A	409	HIS

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Mol	Chain	Res	Type
1	A	413	HIS
1	A	418	ASN
1	A	430	ASN
1	A	522	ASN
1	A	553	ASN
1	A	690	HIS
1	A	692	ASN

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

12 carbohydrates 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	PA1	A	1000	8,2,7	11,11,12	2.64	4 (36%)	11,15,17	2.31	5 (45%)
2	GCN	A	1001	3,2,7	10,10,11	1.85	3 (30%)	10,13,15	2.55	2 (20%)
2	FTT	A	1004	2,7	14,15,16	0.52	0	15,15,17	2.08	2 (13%)
2	KDO	A	1008	2	12,15,16	0.93	0	12,21,24	0.85	0
2	KDO	A	1009	2	12,15,16	0.54	0	12,21,24	0.76	0
2	GMH	A	1010	8,2	13,13,14	0.77	0	17,18,20	1.41	4 (23%)
2	GMH	A	1011	3,2	13,13,14	0.94	1 (7%)	17,18,20	1.12	2 (11%)
2	GMH	A	1012	2	13,13,14	0.48	0	17,18,20	0.98	2 (11%)
2	GLC	A	1017	2	11,11,12	0.56	0	14,15,17	1.07	2 (14%)
2	GLC	A	1018	2	11,11,12	0.52	0	14,15,17	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLA	A	1019	2	11,11,12	0.45	0	14,15,17	0.56	0
2	GLC	A	1020	2	11,11,12	0.52	0	14,15,17	0.63	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	PA1	A	1000	8,2,7	-	0/2/18/22	0/1/1/1
2	GCN	A	1001	3,2,7	1/1/3/4	0/2/15/18	0/1/1/1
2	FTT	A	1004	2,7	-	0/14/14/15	0/0/0/0
2	KDO	A	1008	2	-	0/6/26/30	0/1/1/1
2	KDO	A	1009	2	-	0/6/26/30	0/1/1/1
2	GMH	A	1010	8,2	-	0/6/23/26	0/1/1/1
2	GMH	A	1011	3,2	2/2/5/6	0/6/23/26	0/1/1/1
2	GMH	A	1012	2	2/2/5/6	0/6/23/26	0/1/1/1
2	GLC	A	1017	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1018	2	-	0/2/19/22	0/1/1/1
2	GLA	A	1019	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1020	2	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	PA1	C3-C4	-4.20	1.46	1.52
2	A	1001	GCN	C1-C2	-2.78	1.48	1.52
2	A	1011	GMH	O5-C5	2.09	1.46	1.43
2	A	1000	PA1	O5-C5	2.29	1.50	1.44
2	A	1001	GCN	C3-C4	2.53	1.56	1.52
2	A	1001	GCN	C4-C5	3.89	1.59	1.52
2	A	1000	PA1	O5-C1	4.11	1.50	1.43
2	A	1000	PA1	C1-C2	5.31	1.59	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1004	FTT	O2-C1-C2	-7.30	98.61	125.24
2	A	1000	PA1	C6-C5-C4	-4.19	107.95	113.29
2	A	1000	PA1	C3-C2-C1	-4.12	98.77	109.54
2	A	1000	PA1	O4-C4-C3	-2.20	104.68	110.06
2	A	1000	PA1	O5-C1-C2	-2.12	107.13	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1010	GMH	C1-C2-C3	-2.07	107.10	109.54
2	A	1012	GMH	C1-O5-C5	2.18	115.06	111.52
2	A	1004	FTT	O3-C3-C2	2.23	115.08	109.32
2	A	1010	GMH	C1-O5-C5	2.25	115.17	111.52
2	A	1011	GMH	O5-C5-C6	2.37	109.21	106.04
2	A	1010	GMH	O5-C5-C6	2.48	109.36	106.04
2	A	1017	GLC	C1-C2-C3	2.49	112.49	109.54
2	A	1017	GLC	C1-O5-C5	2.51	115.44	112.25
2	A	1000	PA1	O1-C1-C2	2.53	114.80	109.02
2	A	1012	GMH	O5-C5-C6	2.67	109.61	106.04
2	A	1011	GMH	C1-C2-C3	2.93	113.00	109.54
2	A	1010	GMH	O3-C3-C2	3.15	115.69	110.00
2	A	1001	GCN	C3-C2-N2	3.90	118.16	110.64
2	A	1001	GCN	C3-C2-C1	6.73	116.02	109.60

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	GCN	C1
2	A	1011	GMH	C6
2	A	1011	GMH	C1
2	A	1012	GMH	C6
2	A	1012	GMH	C1

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	1009	KDO	1	0
2	A	1010	GMH	1	0

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	FTT	A	1002	2	14,15,16	0.97	1 (7%)	15,15,17	2.41	2 (13%)
7	FTT	A	1003	2	5,8,16	0.54	0	5,9,17	0.52	0
7	FTT	A	1005	2	12,12,16	0.44	0	10,11,17	0.49	0
7	FTT	A	1006	2,7	13,16,16	0.67	0	13,17,17	0.52	0
7	FTT	A	1007	7	14,14,16	0.47	0	12,13,17	0.59	0
8	DPO	A	1013	2	5,7,8	2.62	3 (60%)	6,10,13	1.52	0
3	PO4	A	1014	2	0,3,4	0.00	-	0,3,6	0.00	-
8	DPO	A	1015	2	5,7,8	2.88	2 (40%)	6,10,13	1.44	0
3	PO4	A	1016	2,4	0,3,4	0.00	-	0,3,6	0.00	-
9	RIF	A	1022	-	66,72,72	2.79	21 (31%)	80,106,106	2.65	22 (27%)
10	DDQ	A	1023	-	13,13,13	1.08	1 (7%)	14,15,15	0.60	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
7	FTT	A	1002	2	1/1/1/2	0/14/14/15	0/0/0/0
7	FTT	A	1003	2	-	0/5/7/15	0/0/0/0
7	FTT	A	1005	2	-	0/9/10/15	0/0/0/0
7	FTT	A	1006	2,7	1/1/2/2	0/13/15/15	0/0/0/0
7	FTT	A	1007	7	-	0/11/12/15	0/0/0/0
8	DPO	A	1013	2	-	0/3/5/6	0/0/0/0
3	PO4	A	1014	2	-	0/0/0/0	0/0/0/0
8	DPO	A	1015	2	-	0/3/5/6	0/0/0/0
3	PO4	A	1016	2,4	-	0/0/0/0	0/0/0/0
9	RIF	A	1022	-	2/2/27/36	0/67/145/145	0/2/6/6
10	DDQ	A	1023	-	-	0/11/11/11	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1022	RIF	C2-C38	-10.32	1.44	1.51
8	A	1015	DPO	P1-O4	-4.31	1.49	1.63
8	A	1015	DPO	P2-O4	-4.08	1.50	1.62
8	A	1013	DPO	P1-O4	-3.72	1.51	1.63
8	A	1013	DPO	P2-O4	-3.63	1.51	1.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1022	RIF	C55-C53	-3.43	1.41	1.49
10	A	1023	DDQ	CM2-N1	-2.51	1.45	1.49
8	A	1013	DPO	P2-O6	-2.09	1.48	1.51
9	A	1022	RIF	O19-C44	2.18	1.39	1.33
9	A	1022	RIF	O6-C20	2.29	1.50	1.43
9	A	1022	RIF	O18-C28	2.33	1.52	1.42
9	A	1022	RIF	C19-C18	2.37	1.60	1.54
7	A	1002	FTT	C5-C4	2.38	1.63	1.52
9	A	1022	RIF	C17-C18	2.49	1.61	1.54
9	A	1022	RIF	O4-C3	2.60	1.27	1.22
9	A	1022	RIF	C52-N6	2.76	1.42	1.36
9	A	1022	RIF	C12-N4	2.86	1.48	1.41
9	A	1022	RIF	C26-N2	2.89	1.52	1.47
9	A	1022	RIF	C51-N6	3.07	1.42	1.36
9	A	1022	RIF	O5-C22	3.11	1.48	1.39
9	A	1022	RIF	C51-C53	3.92	1.40	1.33
9	A	1022	RIF	O7-C18	4.57	1.51	1.44
9	A	1022	RIF	O19-C36	4.73	1.56	1.44
9	A	1022	RIF	C23-C38	5.39	1.50	1.39
9	A	1022	RIF	C12-C1	5.51	1.49	1.39
9	A	1022	RIF	C43-C42	5.56	1.55	1.51
9	A	1022	RIF	C40-C39	7.47	1.45	1.34
9	A	1022	RIF	C41-C42	7.77	1.49	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1002	FTT	O2-C1-C2	-8.56	94.01	125.24
9	A	1022	RIF	C43-C1-C12	-8.04	118.92	123.54
9	A	1022	RIF	C43-C42-C41	-6.37	119.88	123.54
9	A	1022	RIF	O1-C1-C12	-4.04	121.22	124.27
9	A	1022	RIF	O17-C38-C23	-3.44	115.79	124.06
9	A	1022	RIF	C29-N2-C23	-2.84	111.89	121.05
9	A	1022	RIF	C31-C13-C11	-2.36	104.29	110.07
9	A	1022	RIF	C32-C15-C16	-2.29	106.52	111.24
9	A	1022	RIF	C6-C41-C42	-2.24	119.23	122.89
9	A	1022	RIF	C34-C19-C18	-2.21	107.26	111.38
9	A	1022	RIF	O9-C16-C17	-2.17	104.91	109.59
9	A	1022	RIF	C13-C11-C10	2.08	130.72	126.07
9	A	1022	RIF	C36-O19-C44	2.63	121.90	115.96
9	A	1022	RIF	C17-C16-C15	2.70	119.64	115.25
9	A	1022	RIF	O16-C7-N4	2.80	128.47	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1022	RIF	C4-O5-C22	2.85	123.95	116.58
9	A	1022	RIF	C53-C55-C54	2.95	121.32	114.28
7	A	1002	FTT	C4-C3-C2	3.22	122.89	112.23
9	A	1022	RIF	C18-O7-C35	3.76	124.41	117.75
9	A	1022	RIF	C13-C14-C15	3.93	120.68	114.24
9	A	1022	RIF	C12-N4-C7	4.70	136.20	122.98
9	A	1022	RIF	O1-C1-C43	8.01	119.81	112.25
9	A	1022	RIF	O2-C42-C43	8.34	120.13	112.25
9	A	1022	RIF	O17-C38-C2	10.97	122.61	112.25

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1002	FTT	C3
9	A	1022	RIF	C43
9	A	1022	RIF	C2
7	A	1006	FTT	C3

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1002	FTT	8	0
7	A	1005	FTT	2	0
7	A	1006	FTT	7	0
7	A	1007	FTT	5	0
8	A	1015	DPO	1	0
9	A	1022	RIF	4	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	707/707 (100%)	-0.09	8 (1%)	82	80	28, 64, 106, 122	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	GLY	4.5
1	A	101	SER	2.7
1	A	495	TYR	2.4
1	A	113	GLY	2.4
1	A	519	LYS	2.3
1	A	634	PHE	2.3
1	A	118	ASP	2.2
1	A	638	LEU	2.0

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

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

6.3 Carbohydrates

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	FTT	A	1004	16/17	0.92	0.28	4.12	57,65,69,69	1
2	GCN	A	1001	10/11	0.93	0.14	-2.17	35,49,58,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	KDO	A	1008	15/16	0.97	0.12	-2.59	55,62,66,72	0
2	GLC	A	1020	11/12	0.87	0.45	-	122,123,123,123	0
2	KDO	A	1009	15/16	0.90	0.16	-	71,75,82,85	0
2	PA1	A	1000	11/12	0.90	0.15	-	51,63,74,80	0
2	GLC	A	1017	11/12	0.92	0.28	-	90,93,101,103	0
2	GMH	A	1011	13/14	0.91	0.20	-	67,87,102,111	0
2	GLA	A	1019	11/12	0.89	0.28	-	108,108,111,111	0
2	GMH	A	1012	13/14	0.83	0.39	-	116,119,123,123	0
2	GLC	A	1018	11/12	0.90	0.35	-	112,116,119,120	0
2	GMH	A	1010	13/14	0.97	0.12	-	53,62,72,76	0

6.4 Ligands

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
10	DDQ	A	1023	14/14	0.86	0.42	18.35	104,110,122,123	0
7	FTT	A	1007	15/17	0.88	0.45	12.26	72,84,99,100	0
5	NA	A	1024	1/1	0.90	0.46	6.19	102,102,102,102	0
7	FTT	A	1002	16/17	0.89	0.24	3.53	62,67,78,78	0
6	MG	A	1025	1/1	0.79	0.23	2.00	90,90,90,90	0
7	FTT	A	1005	13/17	0.95	0.21	1.97	66,69,72,75	0
9	RIF	A	1022	67/67	0.89	0.29	1.08	81,98,108,110	0
8	DPO	A	1013	8/9	0.96	0.10	-	87,89,92,96	0
4	NI	A	1021	1/1	0.92	0.08	-	95,95,95,95	0
3	PO4	A	1014	4/5	0.93	0.15	-	73,76,80,83	0
7	FTT	A	1003	9/17	0.92	0.27	-	81,95,105,105	0
3	PO4	A	1016	4/5	0.90	0.10	-	91,93,96,98	0
8	DPO	A	1015	8/9	0.96	0.10	-	81,97,108,108	0
7	FTT	A	1006	17/17	0.93	0.32	-	57,76,87,88	0

6.5 Other polymers

There are no such residues in this entry.