Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 07:08 pm GMT

PDB ID	:	4CMQ
Title	:	Crystal structure of Mn-bound S.pyogenes Cas9
Authors	:	Jinek, M.; Jiang, F.; Taylor, D.W.; Sternberg, S.H.; Kaya, E.; Ma, E.; Anders, C.; Hauer, M.; Zhou, K.; Lin, S.; Kaplan, M.; Iavarone, A.T.; Charpentier, E.; Nogales, E.; Doudna, J.A.
Deposited on	:	2014-01-17
Resolution	:	3.09 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 (i) 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 (i)) were used in the production of this report:

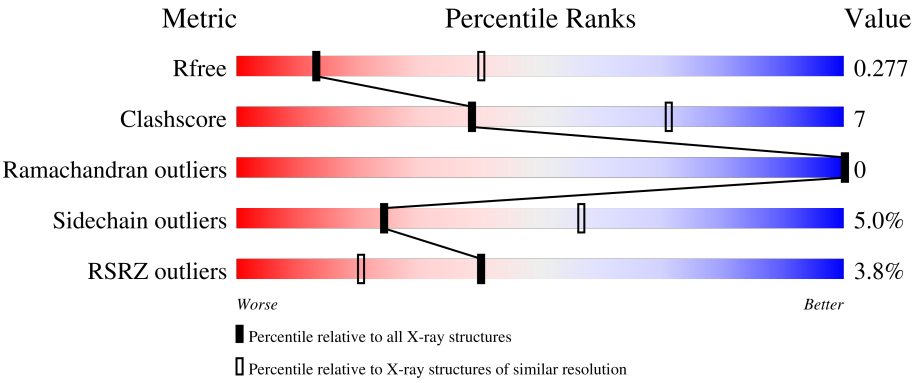
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.09 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	1372	% 67% 17% · 16%
1	B	1372	5% 66% 18% · 15%

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
3	SO4	B	2372	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18904 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 CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1156	Total	C	N	O	S	0	0	0
			9407	6011	1629	1748	19			
1	B	1168	Total	C	N	O	S	0	0	0
			9454	6038	1638	1759	19			

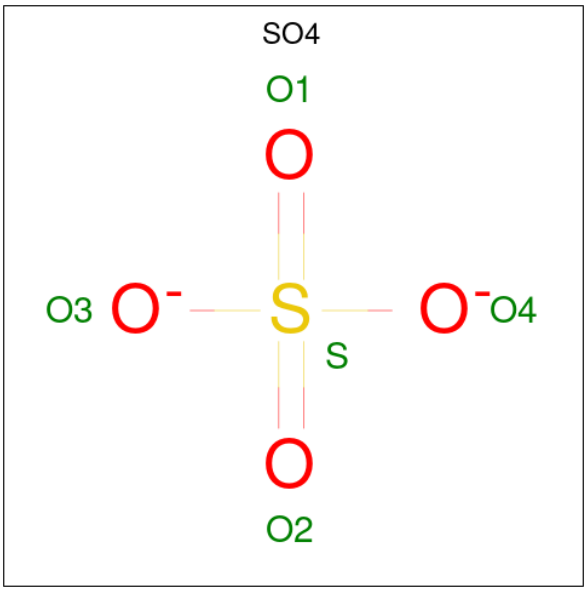
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q99ZW2
A	-2	ALA	-	expression tag	UNP Q99ZW2
A	-1	ALA	-	expression tag	UNP Q99ZW2
A	0	SER	-	expression tag	UNP Q99ZW2
B	-3	GLY	-	expression tag	UNP Q99ZW2
B	-2	ALA	-	expression tag	UNP Q99ZW2
B	-1	ALA	-	expression tag	UNP Q99ZW2
B	0	SER	-	expression tag	UNP Q99ZW2

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Mn	0	0
			7	7		
2	B	6	Total	Mn	0	0
			6	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



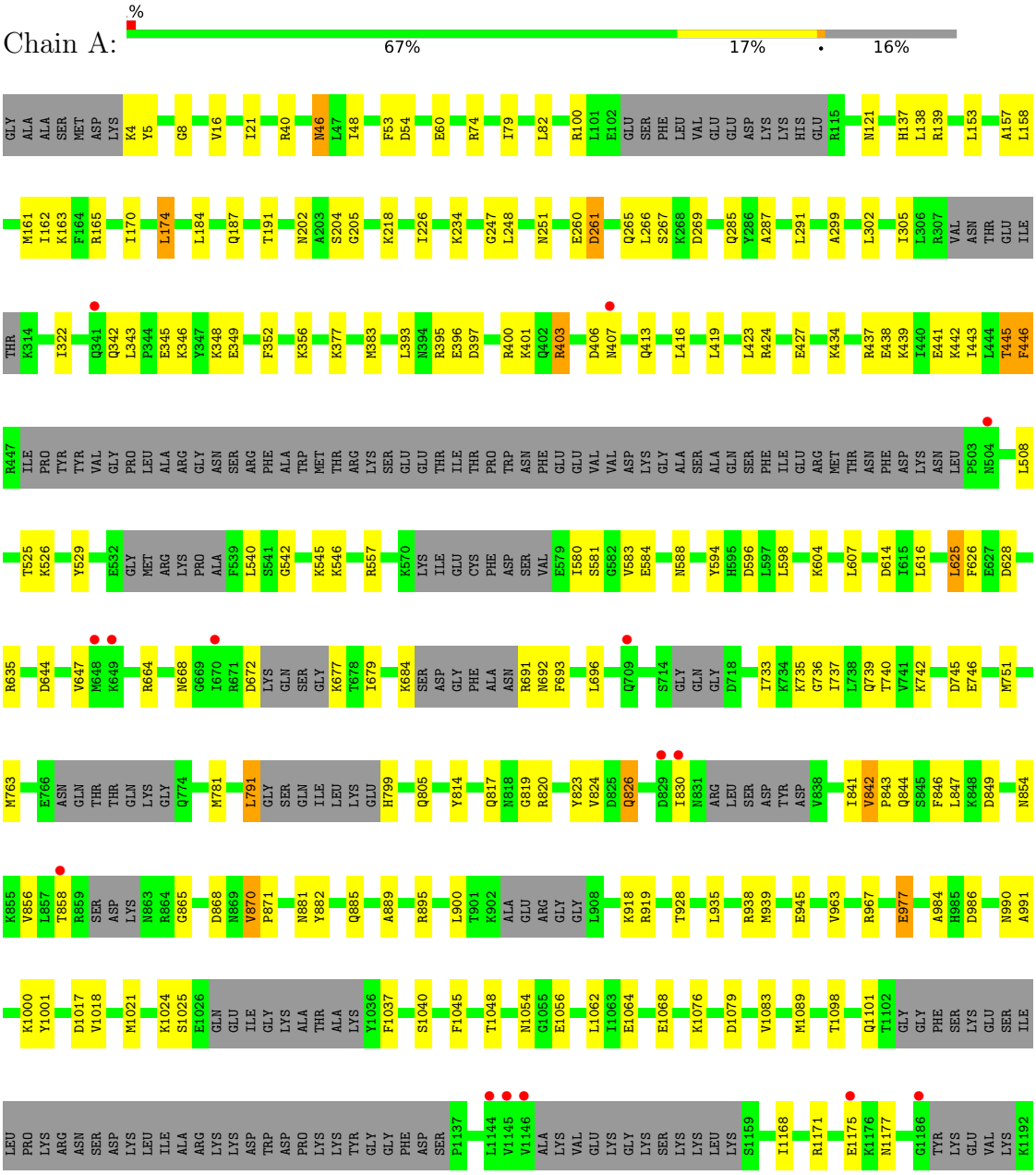
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

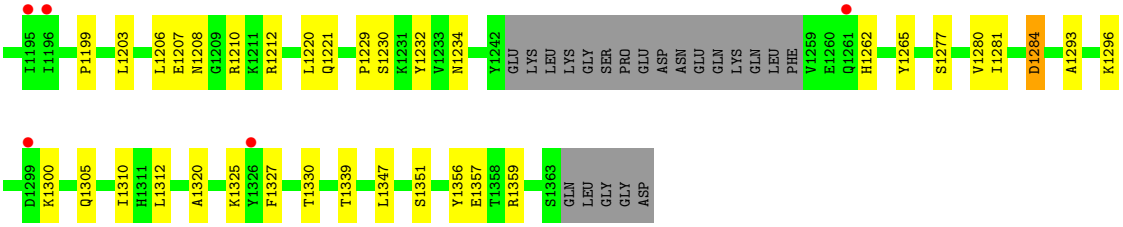
3 Residue-property plots (i)

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.

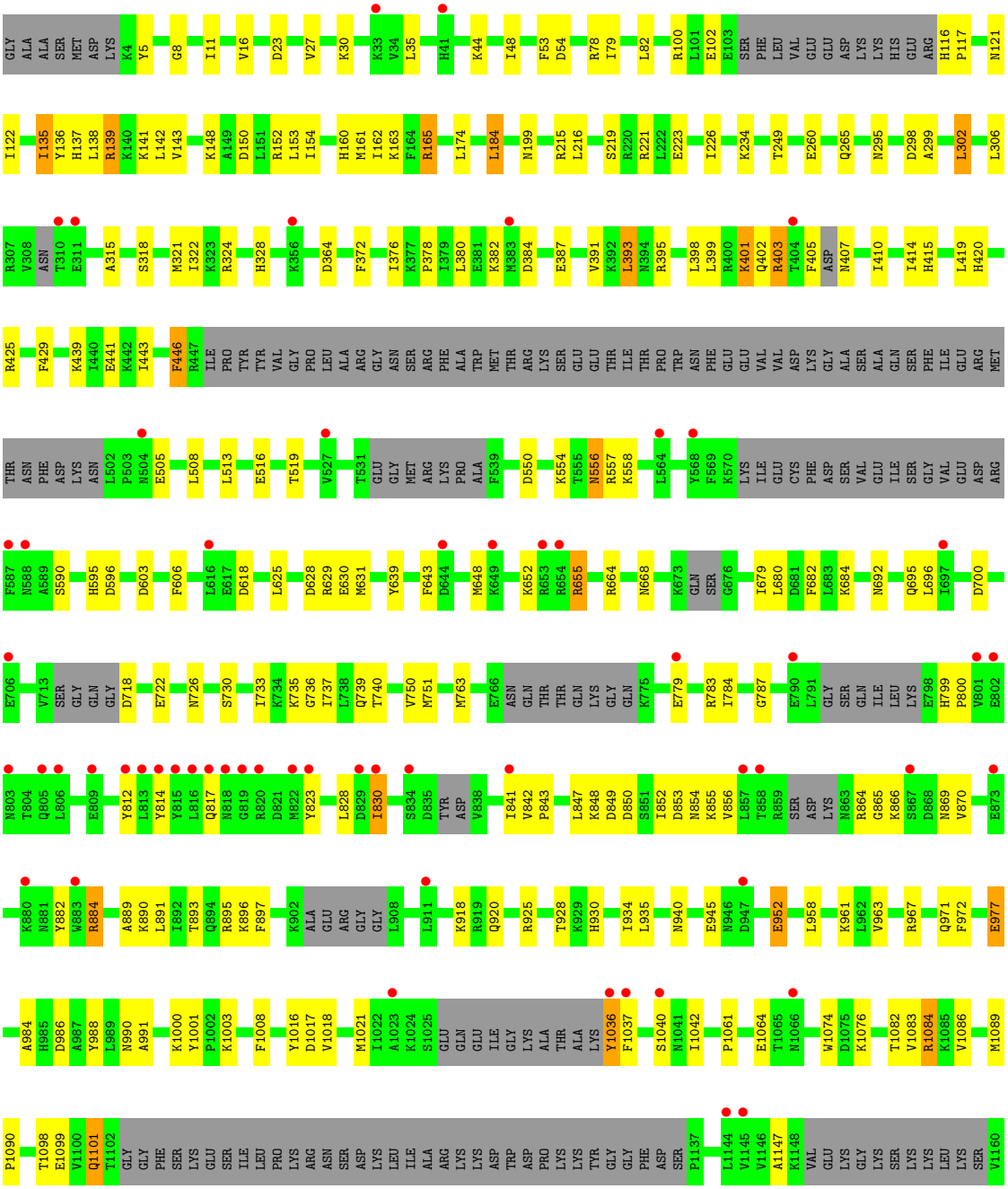
• Molecule 1: CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1

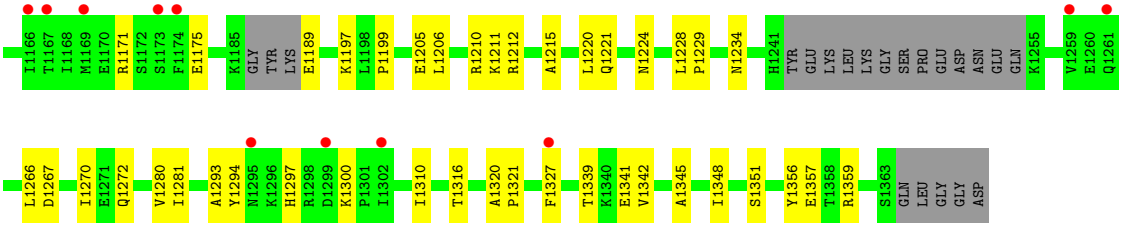
Chain A:





• Molecule 1: CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1




I1166
T1167
I1168
M1169
E1170
R1171
S1172
S1173
F1174
E1175
K1185
GLY
TYR
LYS
E1189
K1197
L1198
P1199
E1205
L1206
R1210
K1211
R1212
A1215
L1220
Q1221
N1224
L1228
P1229
N1234
H1241
TYR
GLU
LYS
LEU
LYS
GLY
SER
PRO
GLU
ASP
ASN
GLU
GLN
K1255
V1259
E1260
Q1261
L1266
D1267
I1270
E1271
Q1272
V1280
I1281
A1293
Y1294
N1295
K1296
H1297
R1298
D1299
K1300
P1301
I1302
I1310
T1316
A1320
P1321
F1327
T1339
K1340
E1341
V1342
A1345
I1348
S1351
Y1356
E1357
T1358
R1359
S1363
GLN
LEU
GLY
GLY
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	159.88Å 210.12Å 90.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.53 – 3.09 47.53 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.53-3.09) 99.0 (47.53-3.09)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 3.07Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.249 , 0.277 0.249 , 0.277	Depositor DCC
R_{free} test set	1500 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å^2)	77.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	18904	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.32% 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: SO4, MN

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	0.24	0/9555	0.43	0/12836
1	B	0.24	0/9601	0.42	0/12909
All	All	0.24	0/19156	0.43	0/25745

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	9407	0	9528	129	0
1	B	9454	0	9536	154	0
2	A	7	0	0	0	0
2	B	6	0	0	0	0
3	A	15	0	0	2	0
3	B	15	0	0	3	0
All	All	18904	0	19064	283	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 7.

All (283) 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:1207:GLU:HG3	1:A:1208:ASN:H	1.04	1.16
1:A:1207:GLU:HG3	1:A:1208:ASN:N	1.84	0.90
1:A:1207:GLU:CG	1:A:1208:ASN:H	1.82	0.84
1:A:184:LEU:HD12	1:A:299:ALA:HB2	1.64	0.79
1:B:967:ARG:NH1	1:B:986:ASP:OD1	2.16	0.78
1:B:1205:GLU:OE1	1:B:1359:ARG:NH2	2.19	0.76
1:A:977:GLU:HG3	1:A:1310:ILE:HG23	1.68	0.73
1:A:247:GLY:HA2	1:A:407:ASN:HB2	1.71	0.73
1:A:349:GLU:HG3	1:A:356:LYS:HD3	1.71	0.73
1:B:1224:ASN:ND2	3:B:2372:SO4:O2	2.23	0.72
1:B:165:ARG:NH2	1:B:446:PHE:O	2.23	0.72
1:B:893:THR:HG23	1:B:896:LYS:H	1.54	0.71
1:B:963:VAL:HG21	1:B:990:ASN:HD22	1.54	0.71
1:B:199:ASN:ND2	1:B:779:GLU:OE1	2.25	0.70
1:B:82:LEU:HD22	1:B:162:ILE:HD12	1.74	0.69
1:B:977:GLU:HG3	1:B:1310:ILE:HG23	1.75	0.69
1:A:598:LEU:HD21	1:A:604:LYS:HG2	1.74	0.69
1:A:343:LEU:HD23	1:A:346:LYS:HD2	1.75	0.68
1:A:100:ARG:NH1	1:A:625:LEU:O	2.27	0.68
1:A:1207:GLU:CG	1:A:1208:ASN:N	2.46	0.67
1:A:158:LEU:HD22	1:A:419:LEU:HD22	1.75	0.67
1:A:1098:THR:HB	1:A:1199:PRO:HB2	1.77	0.66
1:B:1357:GLU:OE2	1:B:1359:ARG:NH1	2.27	0.66
1:B:165:ARG:NH1	3:B:2370:SO4:O4	2.28	0.66
1:B:184:LEU:HD13	1:B:299:ALA:HB2	1.76	0.66
1:A:401:LYS:HB3	1:A:403:ARG:HE	1.59	0.65
1:B:866:LYS:NZ	1:B:870:VAL:O	2.30	0.65
1:B:849:ASP:HB3	1:B:854:ASN:HD22	1.63	0.64
1:B:100:ARG:NH1	1:B:625:LEU:O	2.30	0.64
1:B:787:GLY:HA2	1:B:889:ALA:HB1	1.79	0.64
1:A:967:ARG:NH1	1:A:986:ASP:OD1	2.30	0.64
1:A:174:LEU:HD21	1:A:302:LEU:HD21	1.78	0.64
1:B:848:LYS:O	1:B:961:LYS:NZ	2.31	0.63
1:A:79:ILE:HD11	1:A:163:LYS:HG3	1.82	0.62
1:B:78:ARG:NH1	1:B:162:ILE:O	2.32	0.62
1:A:614:ASP:OD1	1:A:664:ARG:NH2	2.32	0.62
1:A:791:LEU:HD21	1:A:889:ALA:HB2	1.81	0.61
1:B:629:ARG:HG3	1:B:655:ARG:HH12	1.65	0.61
1:B:643:PHE:HD2	1:B:648:MET:HE1	1.65	0.61
1:A:1357:GLU:OE1	1:A:1359:ARG:NH1	2.33	0.61
1:B:380:LEU:HD12	1:B:393:LEU:HD12	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:ASP:OD2	1:A:895:ARG:NH2	2.33	0.61
1:B:79:ILE:HD11	1:B:163:LYS:HG3	1.83	0.60
1:B:410:ILE:HD12	1:B:414:ILE:HD11	1.83	0.60
1:B:8:GLY:HA3	1:B:991:ALA:HB2	1.83	0.60
1:A:427:GLU:HB2	1:A:434:LYS:HB2	1.85	0.59
1:A:817:GLN:O	1:A:882:TYR:OH	2.21	0.59
1:B:1212:ARG:NH2	1:B:1280:VAL:O	2.30	0.59
1:B:249:THR:HG23	1:B:265:GLN:HB2	1.85	0.59
1:A:396:GLU:O	1:A:400:ARG:NH1	2.36	0.58
1:A:1212:ARG:NH2	1:A:1280:VAL:O	2.37	0.58
1:B:1147:ALA:O	1:B:1189:GLU:N	2.37	0.58
1:A:868:ASP:HA	1:A:1054:ASN:HB3	1.86	0.58
1:B:817:GLN:O	1:B:882:TYR:OH	2.21	0.57
1:A:1351:SER:HB2	1:A:1356:TYR:HB2	1.86	0.57
1:B:557:ARG:NH2	1:B:596:ASP:OD1	2.32	0.57
1:B:1293:ALA:O	1:B:1297:HIS:ND1	2.35	0.57
1:B:54:ASP:O	1:B:735:LYS:NZ	2.38	0.56
1:B:652:LYS:O	1:B:655:ARG:NH2	2.38	0.56
1:A:736:GLY:O	1:A:740:THR:HG23	2.04	0.56
1:A:21:ILE:HD12	1:A:991:ALA:HB3	1.87	0.56
1:A:54:ASP:O	1:A:735:LYS:NZ	2.32	0.56
1:B:324:ARG:NH1	1:B:401:LYS:O	2.39	0.56
1:B:722:GLU:O	1:B:726:ASN:ND2	2.39	0.56
1:A:377:LYS:HE2	1:A:393:LEU:HD21	1.88	0.55
1:B:121:ASN:HA	1:B:628:ASP:HB2	1.88	0.55
1:B:226:ILE:HD11	1:B:234:LYS:HG3	1.88	0.55
1:B:11:ILE:HB	1:B:763:MET:HG3	1.86	0.55
1:B:223:GLU:HG2	1:B:234:LYS:HE2	1.88	0.55
1:B:138:LEU:HD11	1:B:153:LEU:HB3	1.89	0.55
1:B:763:MET:O	1:B:925:ARG:NH1	2.39	0.55
1:B:391:VAL:HG12	1:B:395:ARG:HH11	1.72	0.55
1:A:48:ILE:HG12	1:A:984:ALA:HB1	1.89	0.55
1:B:30:LYS:NZ	1:B:750:VAL:O	2.39	0.55
1:B:963:VAL:HG21	1:B:990:ASN:ND2	2.20	0.54
1:A:1284:ASP:N	1:A:1284:ASP:OD1	2.37	0.54
1:B:216:LEU:O	1:B:221:ARG:NH1	2.39	0.54
1:A:60:GLU:OE2	1:A:742:LYS:NZ	2.41	0.54
1:A:139:ARG:NH2	1:A:161:MET:HG2	2.23	0.54
1:B:1211:LYS:N	1:B:1224:ASN:OD1	2.37	0.54
1:B:420:HIS:ND1	1:B:441:GLU:OE2	2.41	0.54
1:B:1084:ARG:HH22	1:B:1234:ASN:HD21	1.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:ASP:OD2	1:A:938:ARG:NH2	2.40	0.53
1:A:138:LEU:HD11	1:A:153:LEU:HB3	1.90	0.53
1:A:1230:SER:O	1:A:1234:ASN:ND2	2.42	0.53
1:B:787:GLY:HA3	1:B:891:LEU:HD21	1.91	0.53
1:B:48:ILE:HG12	1:B:984:ALA:HB1	1.90	0.52
1:B:298:ASP:OD1	1:B:407:ASN:ND2	2.39	0.52
1:A:849:ASP:HB3	1:A:854:ASN:HD22	1.74	0.52
1:A:247:GLY:HA2	1:A:407:ASN:CB	2.39	0.52
1:A:267:SER:HB3	1:A:407:ASN:H	1.74	0.52
1:A:735:LYS:O	1:A:739:GLN:HG2	2.10	0.52
1:B:1061:PRO:O	1:B:1076:LYS:NZ	2.40	0.52
1:B:972:PHE:HE1	1:B:1084:ARG:HG2	1.75	0.52
1:B:378:PRO:O	1:B:382:LYS:HG2	2.10	0.51
1:A:1171:ARG:O	1:A:1175:GLU:HG2	2.09	0.51
1:B:1281:ILE:HD11	1:B:1316:THR:HG22	1.93	0.51
1:A:870:VAL:HG22	1:A:871:PRO:HD2	1.93	0.51
1:B:143:VAL:HG11	1:B:315:ALA:HB2	1.93	0.51
1:B:1064:GLU:OE2	1:B:1076:LYS:NZ	2.43	0.51
1:A:82:LEU:HD22	1:A:162:ILE:HD12	1.92	0.51
1:A:814:TYR:CZ	1:A:830:ILE:HG12	2.46	0.50
1:B:823:TYR:HB3	1:B:865:GLY:HA3	1.92	0.50
1:B:1220:LEU:HG	1:B:1339:THR:HG22	1.93	0.50
1:B:139:ARG:HH22	1:B:415:HIS:CE1	2.29	0.50
1:B:618:ASP:OD2	1:B:639:TYR:OH	2.25	0.50
1:B:679:ILE:HG23	1:B:696:LEU:HD23	1.92	0.50
1:B:1211:LYS:NZ	3:B:2372:SO4:O4	2.44	0.50
1:A:46:ASN:ND2	1:A:1089:MET:SD	2.85	0.50
1:A:226:ILE:HD12	1:A:234:LYS:HA	1.94	0.50
1:B:161:MET:HE1	1:B:419:LEU:N	2.27	0.50
1:B:5:TYR:CZ	1:B:751:MET:HG3	2.47	0.49
1:B:814:TYR:CZ	1:B:830:ILE:HG23	2.47	0.49
1:A:1277:SER:HA	1:A:1281:ILE:HB	1.94	0.49
1:A:1062:LEU:HD12	1:A:1076:LYS:HB2	1.93	0.49
1:A:626:PHE:CE2	1:A:635:ARG:HD2	2.47	0.49
1:B:850:ASP:O	1:B:855:LYS:NZ	2.41	0.49
1:B:139:ARG:HH21	1:B:160:HIS:CE1	2.30	0.49
1:A:187:GLN:O	1:A:191:THR:HG23	2.13	0.49
1:A:442:LYS:O	1:A:446:PHE:HB3	2.13	0.49
1:A:607:LEU:HD23	1:A:616:LEU:HD21	1.95	0.49
1:A:1229:PRO:HD2	1:A:1232:TYR:HD2	1.77	0.48
1:B:556:ASN:N	1:B:556:ASN:OD1	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:ASN:OD1	1:A:1056:GLU:HB2	2.12	0.48
1:B:391:VAL:O	1:B:395:ARG:HD3	2.14	0.48
1:B:1175:GLU:OE2	1:B:1197:LYS:NZ	2.46	0.48
1:A:251:ASN:ND2	1:A:261:ASP:OD1	2.46	0.48
1:A:269:ASP:OD1	1:A:269:ASP:N	2.46	0.48
1:A:692:ASN:OD1	1:A:693:PHE:N	2.47	0.48
1:B:783:ARG:NE	1:B:890:LYS:O	2.46	0.48
1:A:16:VAL:HG23	1:A:53:PHE:HE2	1.79	0.48
1:B:849:ASP:HB3	1:B:854:ASN:ND2	2.27	0.48
1:B:1064:GLU:HB2	1:B:1074:TRP:HB3	1.96	0.48
1:A:170:ILE:O	1:A:413:GLN:NE2	2.45	0.48
1:A:266:LEU:HD12	1:A:407:ASN:HB3	1.96	0.48
1:A:881:ASN:OD1	1:A:885:GLN:NE2	2.47	0.48
1:B:1224:ASN:HB2	1:B:1280:VAL:HG11	1.96	0.48
1:A:423:LEU:HD13	1:A:437:ARG:HG3	1.95	0.47
1:A:679:ILE:HG23	1:A:696:LEU:HD23	1.96	0.47
1:A:733:ILE:O	1:A:737:ILE:HG13	2.14	0.47
1:B:516:GLU:HA	1:B:519:THR:HG22	1.96	0.47
1:B:733:ILE:O	1:B:737:ILE:HG13	2.13	0.47
1:B:852:ILE:HA	1:B:855:LYS:HB2	1.96	0.47
1:A:963:VAL:HG21	1:A:990:ASN:OD1	2.15	0.47
1:B:557:ARG:O	1:B:590:SER:HB2	2.14	0.47
1:B:692:ASN:HB3	1:B:695:GLN:HG3	1.97	0.47
1:B:150:ASP:OD2	1:B:152:ARG:NH2	2.47	0.47
1:B:321:MET:O	1:B:402:GLN:NE2	2.42	0.47
1:B:298:ASP:O	1:B:302:LEU:HB2	2.14	0.47
1:A:814:TYR:CE1	1:A:819:GLY:HA2	2.50	0.47
1:B:735:LYS:O	1:B:739:GLN:HG2	2.14	0.47
1:A:849:ASP:OD2	1:A:919:ARG:NH2	2.48	0.47
1:A:1048:THR:HG22	1:A:1076:LYS:HD3	1.96	0.47
1:A:1168:ILE:O	1:A:1171:ARG:HG2	2.15	0.47
1:B:930:HIS:O	1:B:934:ILE:HG13	2.15	0.47
1:B:398:LEU:HG	1:B:399:LEU:HG	1.96	0.46
1:B:513:LEU:H	1:B:513:LEU:HD12	1.81	0.46
1:B:249:THR:OG1	1:B:265:GLN:OE1	2.30	0.46
1:B:1210:ARG:NH2	1:B:1341:GLU:OE1	2.48	0.46
1:A:583:VAL:HG12	1:A:584:GLU:O	2.15	0.46
1:A:74:ARG:HD2	3:A:2371:SO4:O2	2.16	0.46
1:A:342:GLN:NE2	1:A:383:MET:O	2.43	0.46
1:B:508:LEU:HD21	1:B:664:ARG:HB2	1.98	0.46
1:B:843:PRO:HG2	1:B:869:ASN:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:PHE:HB2	1:B:696:LEU:HD21	1.98	0.46
1:B:1267:ASP:OD1	1:B:1294:TYR:OH	2.31	0.46
1:A:823:TYR:CD2	1:A:858:THR:HG21	2.51	0.46
1:B:439:LYS:O	1:B:443:ILE:HG13	2.16	0.46
1:A:287:ALA:O	1:A:291:LEU:HG	2.16	0.45
1:A:1325:LYS:HG3	1:A:1330:THR:HG22	1.97	0.45
1:B:226:ILE:HD11	1:B:234:LYS:HE3	1.98	0.45
1:B:842:VAL:HA	1:B:843:PRO:HD3	1.73	0.45
1:B:27:VAL:HG12	1:B:1086:VAL:HG22	1.99	0.45
1:B:550:ASP:HA	1:B:554:LYS:HG3	1.99	0.45
1:B:1084:ARG:HH22	1:B:1234:ASN:ND2	2.13	0.45
1:B:174:LEU:HD21	1:B:302:LEU:HD11	1.98	0.45
1:B:1300:LYS:HE2	1:B:1327:PHE:CE1	2.52	0.45
1:A:439:LYS:O	1:A:443:ILE:HG13	2.17	0.44
1:B:184:LEU:HD22	1:B:295:ASN:HB3	1.98	0.44
1:B:557:ARG:HG2	1:B:558:LYS:HG3	2.00	0.44
1:A:1000:LYS:HG3	1:A:1001:TYR:CE1	2.52	0.44
1:B:1101:GLN:H	1:B:1101:GLN:HG2	1.49	0.44
1:B:1215:ALA:HB2	1:B:1221:GLN:HG3	2.00	0.44
1:B:784:ILE:HD11	1:B:812:TYR:CD1	2.52	0.44
1:A:121:ASN:HA	1:A:628:ASP:HB2	1.99	0.44
1:A:525:THR:HA	1:A:545:LYS:HE2	1.99	0.44
1:A:594:TYR:O	1:A:598:LEU:HB2	2.17	0.44
1:B:219:SER:O	1:B:223:GLU:HG3	2.17	0.44
1:B:1351:SER:HB3	1:B:1356:TYR:HB2	1.99	0.44
1:A:1232:TYR:CE1	1:A:1265:TYR:HD2	2.36	0.44
1:A:1220:LEU:HG	1:A:1339:THR:HG22	1.98	0.44
1:B:5:TYR:CE2	1:B:751:MET:HG3	2.52	0.44
1:B:814:TYR:HE2	1:B:828:LEU:O	2.00	0.44
1:B:1082:THR:O	1:B:1086:VAL:HG23	2.18	0.44
1:A:542:GLY:O	1:A:546:LYS:HG3	2.18	0.44
1:A:918:LYS:HE3	1:A:1018:VAL:HG11	1.99	0.44
1:A:508:LEU:HD21	1:A:664:ARG:HB2	2.00	0.43
1:A:526:LYS:HE3	1:A:692:ASN:HB2	2.00	0.43
1:B:847:LEU:HD12	1:B:848:LYS:N	2.33	0.43
1:B:1098:THR:HB	1:B:1199:PRO:HB2	2.00	0.43
1:B:401:LYS:HB3	1:B:403:ARG:HE	1.83	0.43
1:B:1205:GLU:HB2	1:B:1348:ILE:HD11	1.99	0.43
1:A:403:ARG:NH2	3:A:2372:SO4:O2	2.34	0.43
1:A:1045:PHE:O	1:A:1064:GLU:HG3	2.18	0.43
1:B:1000:LYS:HG3	1:B:1001:TYR:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:VAL:HA	1:A:843:PRO:HD3	1.79	0.43
1:B:16:VAL:HG23	1:B:53:PHE:HE1	1.82	0.43
1:A:557:ARG:NH2	1:A:596:ASP:OD1	2.50	0.43
1:B:382:LYS:HA	1:B:382:LYS:HD3	1.92	0.43
1:A:218:LYS:HB2	1:A:248:LEU:HD21	2.00	0.43
1:A:895:ARG:NH2	1:A:919:ARG:HH22	2.16	0.43
1:A:137:HIS:HA	1:A:322:ILE:HD11	2.00	0.43
1:A:202:ASN:OD1	1:A:204:SER:HB3	2.19	0.43
1:A:583:VAL:CG1	1:A:584:GLU:N	2.82	0.43
1:A:841:ILE:HD13	1:A:900:LEU:HG	2.00	0.43
1:A:856:VAL:HG12	1:A:858:THR:HG23	1.99	0.42
1:B:1206:LEU:HD21	1:B:1345:ALA:HB2	2.01	0.42
1:A:5:TYR:CZ	1:A:751:MET:HG3	2.54	0.42
1:A:1280:VAL:HG23	1:A:1281:ILE:HD12	2.01	0.42
1:B:122:ILE:HG12	1:B:631:MET:HG3	2.01	0.42
1:B:784:ILE:HD11	1:B:812:TYR:HD1	1.85	0.42
1:A:265:GLN:HG2	1:A:407:ASN:OD1	2.19	0.42
1:B:139:ARG:CZ	1:B:161:MET:HG2	2.50	0.42
1:B:410:ILE:HD11	1:B:415:HIS:CE1	2.54	0.42
1:B:763:MET:HB3	1:B:928:THR:HG22	2.01	0.42
1:A:644:ASP:HB2	1:A:647:VAL:HG23	2.01	0.42
1:A:823:TYR:HB3	1:A:865:GLY:HA3	2.00	0.42
1:B:137:HIS:HA	1:B:322:ILE:HD11	2.01	0.42
1:B:1021:MET:O	1:B:1036:TYR:N	2.52	0.42
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.83	0.42
1:A:1024:LYS:HG2	1:A:1025:SER:H	1.84	0.42
1:A:348:LYS:HA	1:A:352:PHE:HD2	1.85	0.42
1:B:161:MET:HE2	1:B:419:LEU:HB2	2.01	0.42
1:B:841:ILE:HD11	1:B:896:LYS:HE3	1.99	0.42
1:A:546:LYS:HE2	1:A:684:LYS:HG2	2.02	0.42
1:A:824:VAL:HB	1:A:826:GLN:HG2	2.02	0.42
1:B:1266:LEU:O	1:B:1270:ILE:HG12	2.19	0.42
1:A:672:ASP:H	1:A:677:LYS:N	2.17	0.42
1:A:763:MET:HB2	1:A:928:THR:HG22	2.02	0.42
1:B:1089:MET:HA	1:B:1090:PRO:HD2	1.86	0.41
1:A:8:GLY:HA3	1:A:991:ALA:HB2	2.02	0.41
1:B:8:GLY:CA	1:B:991:ALA:HB2	2.49	0.41
1:B:136:TYR:HA	1:B:139:ARG:HB2	2.02	0.41
1:B:410:ILE:HD11	1:B:415:HIS:NE2	2.35	0.41
1:B:920:GLN:NE2	1:B:1042:ILE:HG12	2.34	0.41
1:B:1320:ALA:HA	1:B:1321:PRO:HD3	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:LEU:HD23	1:A:607:LEU:HD12	2.02	0.41
1:B:603:ASP:OD1	1:B:606:PHE:N	2.49	0.41
1:A:204:SER:OG	1:A:205:GLY:N	2.53	0.41
1:A:583:VAL:HG12	1:A:584:GLU:N	2.35	0.41
1:A:625:LEU:HD12	1:A:625:LEU:HA	1.87	0.41
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.93	0.41
1:B:318:SER:O	1:B:322:ILE:HG13	2.20	0.41
1:B:799:HIS:HA	1:B:800:PRO:HD2	1.97	0.41
1:A:423:LEU:HD23	1:A:423:LEU:HA	1.82	0.41
1:A:1300:LYS:HD3	1:A:1327:PHE:CE1	2.55	0.41
1:B:116:HIS:HA	1:B:117:PRO:HD3	1.91	0.41
1:B:135:ILE:HG21	1:B:160:HIS:CD2	2.56	0.41
1:B:142:LEU:HD13	1:B:154:ILE:HA	2.02	0.41
1:B:372:PHE:CZ	1:B:376:ILE:HD13	2.56	0.41
1:A:157:ALA:O	1:A:161:MET:HG3	2.20	0.41
1:A:302:LEU:HD12	1:A:305:ILE:HD11	2.03	0.41
1:A:626:PHE:HE2	1:A:635:ARG:HD2	1.86	0.41
1:A:1221:GLN:NE2	1:A:1320:ALA:HB2	2.35	0.41
1:A:1262:HIS:HB3	1:A:1265:TYR:CD1	2.56	0.41
1:B:328:HIS:CE1	1:B:399:LEU:HB3	2.56	0.41
1:B:680:LEU:HG	1:B:684:LYS:HE3	2.01	0.41
1:A:529:TYR:HA	1:A:580:ILE:HA	2.03	0.41
1:A:846:PHE:O	1:A:1040:SER:HB2	2.21	0.41
1:A:1079:ASP:O	1:A:1083:VAL:HG23	2.21	0.41
1:A:1203:LEU:O	1:A:1347:LEU:HD12	2.19	0.41
1:A:1293:ALA:HA	1:A:1296:LYS:HD2	2.03	0.41
1:B:148:LYS:HB2	1:B:429:PHE:CD2	2.57	0.40
1:B:557:ARG:HA	1:B:595:HIS:CD2	2.57	0.40
1:B:730:SER:O	1:B:733:ILE:HG22	2.22	0.40
1:B:884:ARG:HD2	1:B:897:PHE:CZ	2.56	0.40
1:B:940:ASN:OD1	1:B:952:GLU:N	2.54	0.40
1:B:1003:LYS:HD2	1:B:1016:TYR:CE2	2.57	0.40
1:A:441:GLU:O	1:A:445:THR:OG1	2.38	0.40
1:B:736:GLY:O	1:B:740:THR:HG22	2.22	0.40
1:B:988:TYR:HE2	1:B:1083:VAL:HG13	1.86	0.40
1:B:918:LYS:HE2	1:B:1018:VAL:HG11	2.02	0.40
1:B:1228:LEU:HA	1:B:1229:PRO:HD3	1.94	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	1118/1372 (82%)	1088 (97%)	30 (3%)	0	100	100
1	B	1130/1372 (82%)	1104 (98%)	26 (2%)	0	100	100
All	All	2248/2744 (82%)	2192 (98%)	56 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1026/1228 (84%)	976 (95%)	50 (5%)	25	57
1	B	1026/1228 (84%)	974 (95%)	52 (5%)	24	56
All	All	2052/2456 (84%)	1950 (95%)	102 (5%)	24	57

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	40	ARG
1	A	46	ASN
1	A	165	ARG
1	A	174	LEU
1	A	260	GLU
1	A	261	ASP
1	A	285	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	345	GLU
1	A	395	ARG
1	A	397	ASP
1	A	403	ARG
1	A	406	ASP
1	A	416	LEU
1	A	424	ARG
1	A	438	GLU
1	A	445	THR
1	A	446	PHE
1	A	540	LEU
1	A	581	SER
1	A	588	ASN
1	A	625	LEU
1	A	668	ASN
1	A	691	ARG
1	A	746	GLU
1	A	781	MET
1	A	791	LEU
1	A	799	HIS
1	A	805	GLN
1	A	820	ARG
1	A	826	GLN
1	A	842	VAL
1	A	844	GLN
1	A	847	LEU
1	A	870	VAL
1	A	935	LEU
1	A	939	MET
1	A	945	GLU
1	A	977	GLU
1	A	1017	ASP
1	A	1021	MET
1	A	1037	PHE
1	A	1068	GLU
1	A	1101	GLN
1	A	1177	ASN
1	A	1206	LEU
1	A	1210	ARG
1	A	1284	ASP
1	A	1305	GLN
1	A	1312	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	23	ASP
1	B	35	LEU
1	B	44	LYS
1	B	102	GLU
1	B	135	ILE
1	B	139	ARG
1	B	141	LYS
1	B	165	ARG
1	B	184	LEU
1	B	215	ARG
1	B	260	GLU
1	B	302	LEU
1	B	306	LEU
1	B	364	ASP
1	B	384	ASP
1	B	387	GLU
1	B	393	LEU
1	B	401	LYS
1	B	403	ARG
1	B	405	PHE
1	B	425	ARG
1	B	446	PHE
1	B	505	GLU
1	B	556	ASN
1	B	630	GLU
1	B	655	ARG
1	B	668	ASN
1	B	700	ASP
1	B	718	ASP
1	B	830	ILE
1	B	853	ASP
1	B	856	VAL
1	B	864	ARG
1	B	884	ARG
1	B	895	ARG
1	B	935	LEU
1	B	945	GLU
1	B	952	GLU
1	B	958	LEU
1	B	971	GLN
1	B	977	GLU
1	B	1008	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1017	ASP
1	B	1036	TYR
1	B	1037	PHE
1	B	1040	SER
1	B	1084	ARG
1	B	1099	GLU
1	B	1101	GLN
1	B	1171	ARG
1	B	1272	GLN
1	B	1342	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	HIS
1	B	199	ASN
1	B	980	ASN
1	B	990	ASN
1	B	1054	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 13 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	SO4	A	2373	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	B	2370	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	A	2371	-	4,4,4	0.13	0	6,6,6	0.06	0
3	SO4	B	2372	-	4,4,4	0.11	0	6,6,6	0.17	0
3	SO4	A	2372	-	4,4,4	0.13	0	6,6,6	0.05	0
3	SO4	B	2371	-	4,4,4	0.14	0	6,6,6	0.05	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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2370	SO4	1	0
3	A	2371	SO4	1	0
3	B	2372	SO4	2	0
3	A	2372	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1156/1372 (84%)	0.09	20 (1%)	70	49	13, 54, 96, 149	0
1	B	1168/1372 (85%)	0.28	69 (5%)	22	10	12, 61, 113, 147	0
All	All	2324/2744 (84%)	0.19	89 (3%)	40	20	12, 57, 106, 149	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	817	GLN	7.0
1	A	407	ASN	6.2
1	B	830	ILE	5.3
1	B	806	LEU	5.2
1	B	813	LEU	4.7
1	B	815	TYR	4.0
1	B	1169	MET	3.8
1	B	816	LEU	3.7
1	B	1023	ALA	3.7
1	B	829	ASP	3.6
1	B	1302	ILE	3.5
1	A	1299	ASP	3.5
1	B	801	VAL	3.5
1	B	1173	SER	3.4
1	B	1040	SER	3.4
1	B	790	GLU	3.3
1	A	341	GLN	3.1
1	B	834	SER	3.1
1	B	564	LEU	3.1
1	A	504	ASN	3.0
1	B	823	TYR	2.9
1	B	1144	LEU	2.9
1	B	504	ASN	2.9
1	B	568	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1195	ILE	2.8
1	B	33	LYS	2.7
1	A	709	GLN	2.7
1	B	310	THR	2.7
1	B	819	GLY	2.7
1	B	911	LEU	2.7
1	B	802	GLU	2.7
1	A	1326	TYR	2.7
1	B	644	ASP	2.6
1	B	822	MET	2.6
1	B	1166	ILE	2.6
1	B	805	GLN	2.6
1	A	649	LYS	2.5
1	B	857	LEU	2.5
1	B	1145	VAL	2.5
1	B	841	ILE	2.5
1	B	653	ARG	2.5
1	B	818	ASN	2.5
1	A	1261	GLN	2.5
1	A	1144	LEU	2.4
1	B	1299	ASP	2.4
1	A	1146	VAL	2.4
1	B	809	GLU	2.4
1	B	814	TYR	2.4
1	B	1036	TYR	2.4
1	A	1145	VAL	2.4
1	B	1174	PHE	2.4
1	B	1066	ASN	2.4
1	A	830	ILE	2.4
1	B	697	ILE	2.4
1	B	616	LEU	2.3
1	A	858	THR	2.3
1	B	404	THR	2.3
1	B	706	GLU	2.3
1	B	587	PHE	2.3
1	A	1196	ILE	2.3
1	B	588	ASN	2.3
1	B	803	ASN	2.3
1	A	670	ILE	2.3
1	B	527	VAL	2.2
1	B	880	LYS	2.2
1	B	883	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	858	THR	2.2
1	A	829	ASP	2.2
1	B	947	ASP	2.2
1	A	648	MET	2.2
1	B	1295	ASN	2.1
1	B	356	LYS	2.1
1	B	383	MET	2.1
1	B	649	LYS	2.1
1	B	1167	THR	2.1
1	B	779	GLU	2.1
1	B	41	HIS	2.1
1	B	1327	PHE	2.1
1	A	1186	GLY	2.1
1	A	1175	GLU	2.1
1	B	311	GLU	2.1
1	B	654	ARG	2.1
1	B	873	GLU	2.1
1	B	1261	GLN	2.0
1	B	1037	PHE	2.0
1	B	812	TYR	2.0
1	B	1259	VAL	2.0
1	B	820	ARG	2.0
1	B	867	SER	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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	B	2367	1/1	0.59	0.15	96,96,96,96	0
2	MN	A	2369	1/1	0.68	0.20	104,104,104,104	0
3	SO4	A	2373	5/5	0.69	0.26	100,100,102,103	0
2	MN	A	2368	1/1	0.73	0.24	136,136,136,136	0
2	MN	A	2367	1/1	0.81	0.29	84,84,84,84	0
3	SO4	B	2371	5/5	0.83	0.39	111,112,112,112	0
2	MN	B	2368	1/1	0.86	0.17	98,98,98,98	0
2	MN	B	2366	1/1	0.87	0.16	98,98,98,98	0
3	SO4	A	2372	5/5	0.88	0.47	122,123,123,124	0
2	MN	A	2364	1/1	0.89	0.22	31,31,31,31	0
2	MN	A	2370	1/1	0.89	0.23	98,98,98,98	0
3	SO4	B	2372	5/5	0.89	0.18	87,87,89,89	0
2	MN	B	2364	1/1	0.93	0.22	30,30,30,30	0
2	MN	A	2366	1/1	0.93	0.17	53,53,53,53	0
2	MN	A	2365	1/1	0.94	0.18	36,36,36,36	0
2	MN	B	2365	1/1	0.96	0.28	38,38,38,38	0
3	SO4	B	2370	5/5	0.97	0.17	46,48,49,50	0
2	MN	B	2369	1/1	0.97	0.17	69,69,69,69	0
3	SO4	A	2371	5/5	0.97	0.16	36,41,42,43	0

6.5 Other polymers (i)

There are no such residues in this entry.