Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:32 PM GMT

PDB ID	:	4CEH
Title	:	Crystal structure of AddAB with a forked DNA substrate
Authors	:	Krajewski, W.W.; Wilkinson, M.; Fu, X.; Cronin, N.B.; Wigley, D.
Deposited on	:	2013-11-11
Resolution	:	3.24 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:

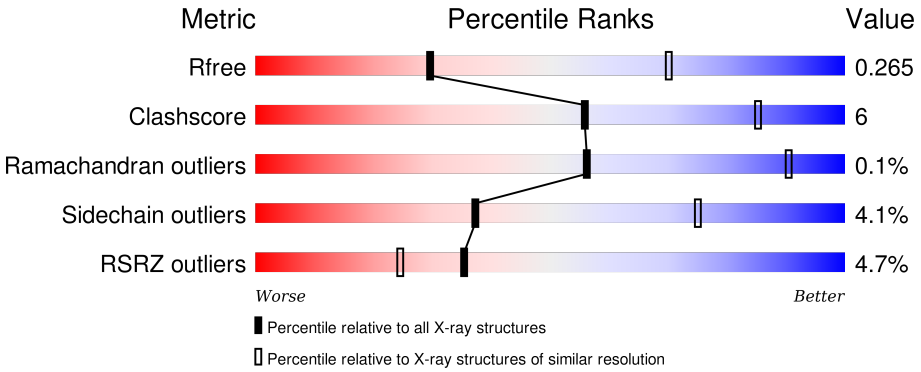
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.24 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	1092 (3.28-3.20)
Clashscore	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RSRZ outliers	91569	1097 (3.28-3.20)

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	1232	3%, 76%, 17%, 6%
2	B	1166	5%, 79%, 18%
3	X	65	20%, 31%, 26%, 43%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19433 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 ATP-DEPENDENT HELICASE/NUCLEASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1154	Total	C	N	O	S	0	0	0
			9339	5966	1589	1757	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	780	GLY	ALA	VARIANT	UNP P23478
A	1172	ALA	ASP	ENGINEERED MUTATION	UNP P23478

- Molecule 2 is a protein called ATP-DEPENDENT HELICASE/DEOXYRIBONUCLEASE SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1148	Total	C	N	O	S	0	0	0
			9330	5929	1597	1760	44			

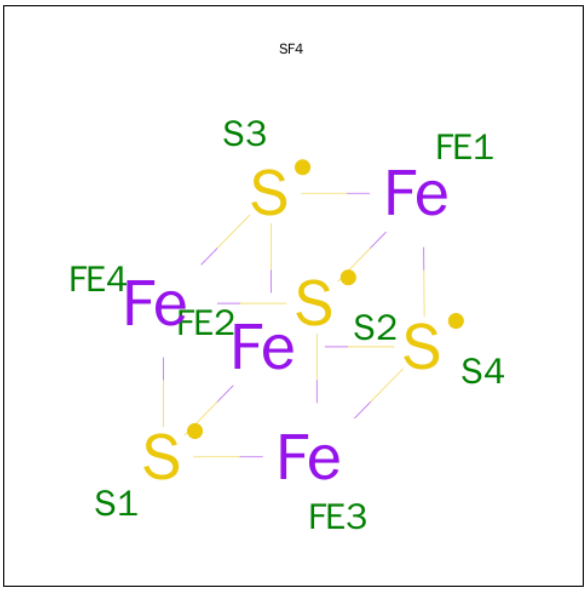
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	843	ASP	GLU	VARIANT	UNP P23477
B	844	GLU	GLN	VARIANT	UNP P23477
B	961	ALA	ASP	ENGINEERED MUTATION	UNP P23477

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	37	Total	C	N	O	P	0	0	0
			756	363	126	230	37			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



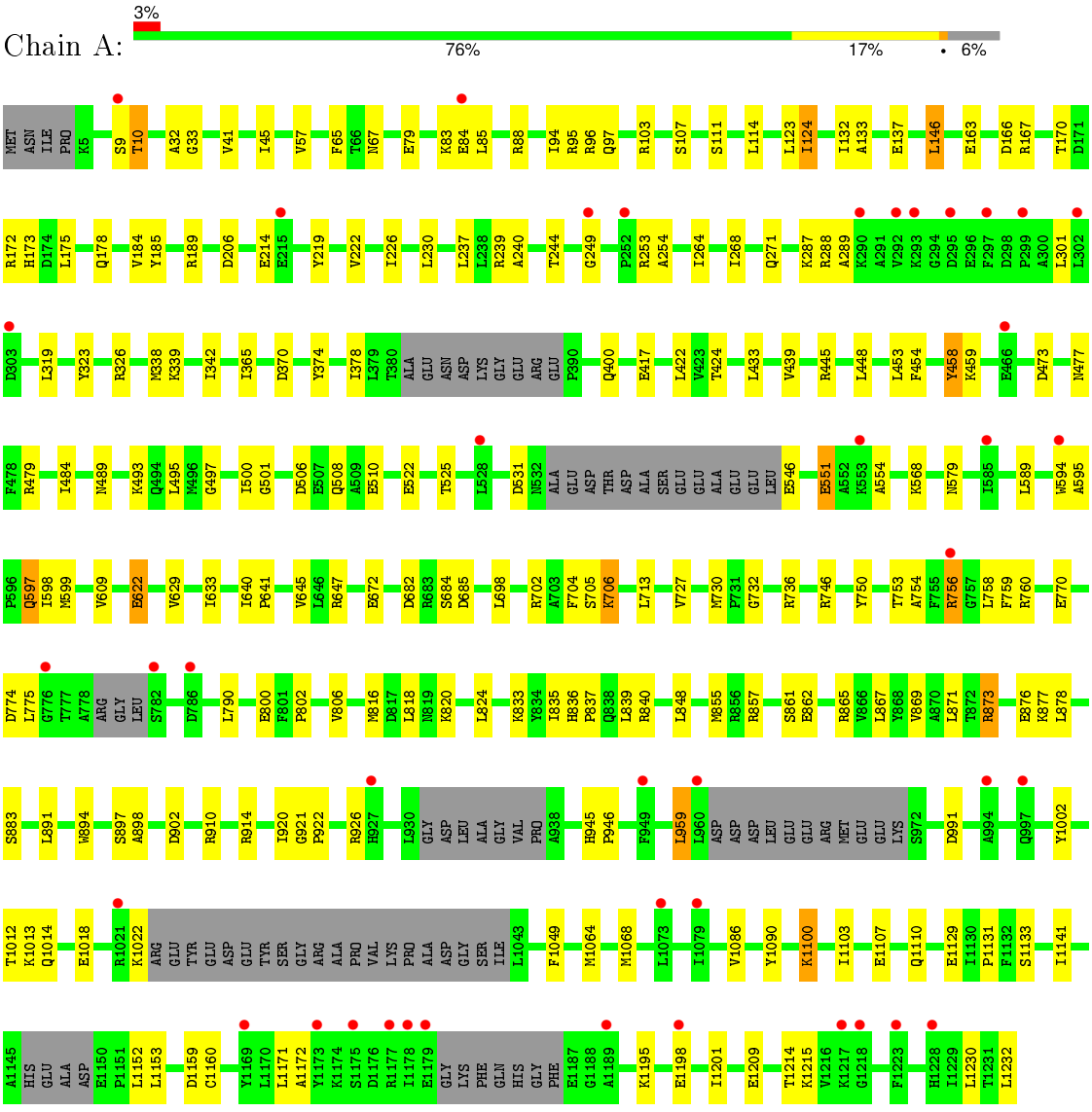
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	B	1	8	4	4	0	0

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.

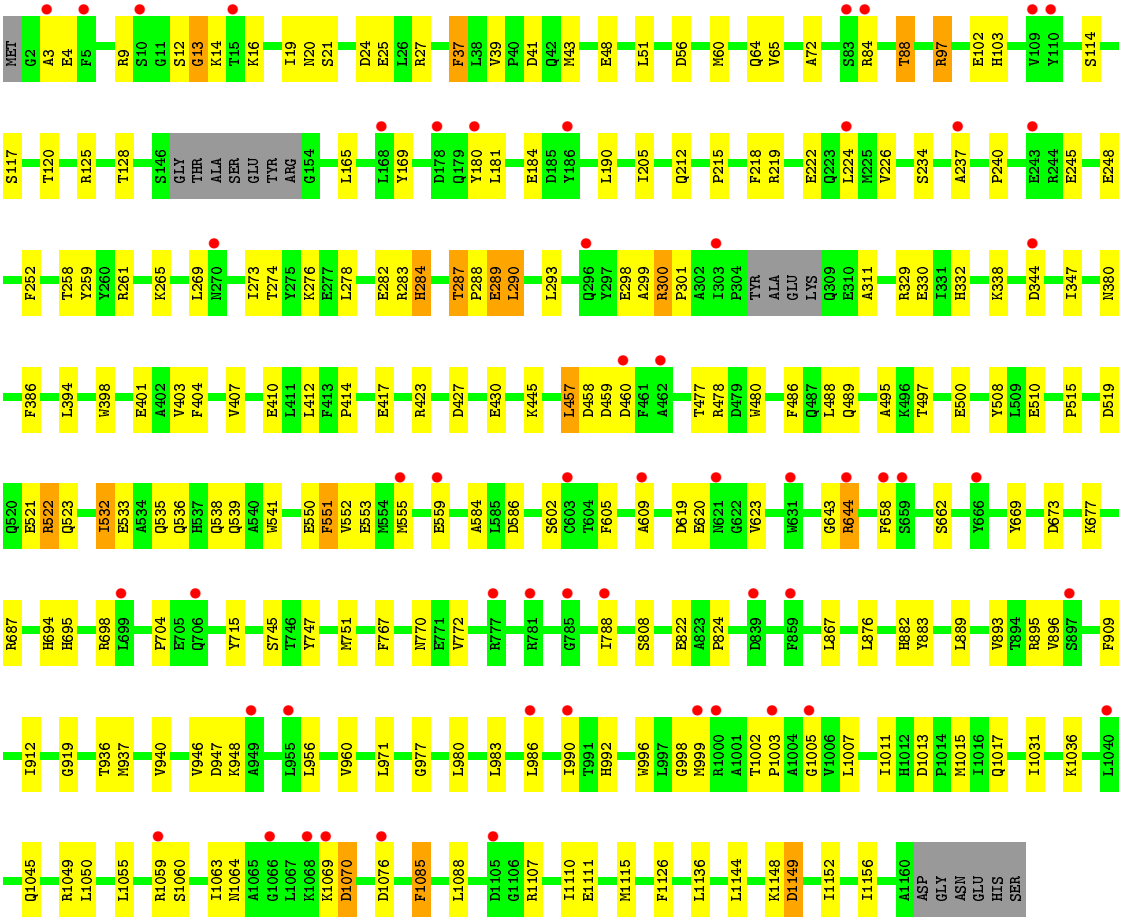
- Molecule 1: ATP-DEPENDENT HELICASE/NUCLEASE SUBUNIT A

Chain A:



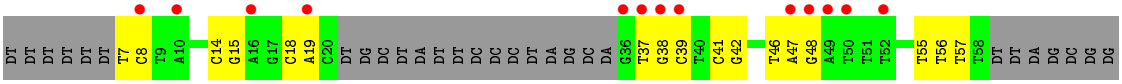
- Molecule 2: ATP-DEPENDENT HELICASE/DEOXYRIBONUCLEASE SUBUNIT B

Chain B:



- Molecule 3: DNA

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	77.37Å 96.77Å 109.69Å 104.38° 96.11° 90.03°	Depositor
Resolution (Å)	29.94 – 3.24 39.52 – 3.24	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.94-3.24) 90.1 (39.52-3.24)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 3.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.229 , 0.264 0.233 , 0.265	Depositor DCC
R_{free} test set	2376 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	96.4	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 68.5	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 47632 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19433	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: SF4

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	0.22	0/9524	0.38	0/12849
2	B	0.22	0/9518	0.38	0/12824
3	X	0.56	0/843	1.04	0/1297
All	All	0.24	0/19885	0.44	0/26970

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	9339	0	9335	121	0
2	B	9330	0	9280	123	0
3	X	756	0	424	13	0
4	B	8	0	0	0	0
All	All	19433	0	19039	238	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (238) 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)
2:B:284:HIS:HB3	2:B:290:LEU:HB3	1.64	0.76
1:A:287:LYS:NZ	3:X:19:DA:OP1	2.20	0.75
2:B:896:VAL:HG21	2:B:1011:ILE:HG23	1.73	0.71
1:A:1090:TYR:HB2	1:A:1100:LYS:HG3	1.73	0.70
1:A:167:ARG:NH1	1:A:835:ILE:O	2.24	0.69
1:A:88:ARG:HD2	1:A:94:ILE:HG13	1.73	0.69
1:A:1013:LYS:NZ	2:B:48:GLU:OE1	2.28	0.66
2:B:245:GLU:OE2	2:B:261:ARG:NH2	2.28	0.65
1:A:79:GLU:OE2	1:A:83:LYS:NZ	2.30	0.65
2:B:1070:ASP:OD1	2:B:1070:ASP:N	2.22	0.65
2:B:445:LYS:O	2:B:478:ARG:NH2	2.29	0.65
1:A:836:HIS:HD2	1:A:839:LEU:H	1.45	0.64
1:A:170:THR:HG23	1:A:172:ARG:H	1.62	0.64
2:B:788:ILE:HB	2:B:937:MET:HG2	1.79	0.64
1:A:96:ARG:HD2	2:B:644:ARG:HH22	1.62	0.64
2:B:300:ARG:H	2:B:300:ARG:HD3	1.63	0.64
2:B:212:GLN:HA	2:B:258:THR:HG21	1.78	0.64
2:B:414:PRO:HB2	2:B:417:GLU:HG3	1.81	0.63
2:B:165:LEU:HD11	2:B:623:VAL:HG11	1.78	0.63
2:B:97:ARG:NH2	2:B:114:SER:O	2.32	0.62
2:B:909:PHE:HB3	2:B:947:ASP:HB3	1.81	0.62
2:B:386:PHE:HE1	2:B:412:LEU:HG	1.65	0.62
2:B:4:GLU:HG3	2:B:274:THR:HB	1.82	0.61
2:B:289:GLU:OE1	2:B:695:HIS:NE2	2.27	0.61
2:B:248:GLU:OE1	2:B:644:ARG:NH1	2.33	0.61
1:A:163:GLU:OE1	1:A:167:ARG:NH2	2.34	0.61
2:B:1045:GLN:HE21	2:B:1049:ARG:HD2	1.66	0.61
1:A:622:GLU:OE2	1:A:736:ARG:NH1	2.34	0.60
1:A:253:ARG:HE	1:A:289:ALA:HB1	1.66	0.60
1:A:554:ALA:HB2	1:A:959:LEU:HD21	1.83	0.59
2:B:300:ARG:HG2	2:B:301:PRO:HD3	1.83	0.59
2:B:497:THR:HA	2:B:559:GLU:HA	1.84	0.58
2:B:1149:ASP:N	2:B:1149:ASP:OD1	2.37	0.58
2:B:410:GLU:OE2	2:B:423:ARG:NH1	2.34	0.58
2:B:13:GLY:N	2:B:282:GLU:OE1	2.35	0.58
1:A:682:ASP:OD2	1:A:684:SER:OG	2.20	0.57
2:B:12:SER:O	2:B:14:LYS:N	2.37	0.57
1:A:898:ALA:HB1	1:A:926:ARG:HG3	1.86	0.57
1:A:123:LEU:HD12	1:A:378:ILE:HG23	1.86	0.57
1:A:1160:CYS:HB3	1:A:1171:LEU:HB3	1.85	0.57
1:A:867:LEU:HD21	1:A:920:ILE:HD11	1.85	0.57
1:A:1214:THR:OG1	1:A:1215:LYS:N	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:GLU:OE2	2:B:276:LYS:NZ	2.32	0.56
1:A:484:ILE:HD12	1:A:878:LEU:HD13	1.86	0.56
2:B:990:ILE:HG13	2:B:1003:PRO:HG3	1.87	0.56
1:A:114:LEU:HD13	1:A:132:ILE:HD11	1.86	0.56
2:B:205:ILE:HD13	2:B:224:LEU:HD13	1.86	0.56
1:A:1133:SER:HB3	1:A:1153:LEU:HD11	1.86	0.56
1:A:1209:GLU:HG2	1:A:1215:LYS:HA	1.88	0.56
1:A:759:PHE:HE2	2:B:401:GLU:HG3	1.71	0.56
1:A:704:PHE:HD2	1:A:713:LEU:HD23	1.71	0.56
1:A:424:THR:HG21	1:A:433:LEU:HB2	1.88	0.55
2:B:180:TYR:OH	2:B:553:GLU:OE1	2.24	0.55
2:B:919:GLY:HA3	2:B:940:VAL:HG12	1.89	0.55
2:B:1036:LYS:HE3	2:B:1064:ASN:HA	1.89	0.55
2:B:912:ILE:HD11	2:B:948:LYS:HB3	1.89	0.54
2:B:16:LYS:NZ	2:B:20:ASN:OD1	2.34	0.54
2:B:1059:ARG:NH2	2:B:1076:ASP:OD2	2.38	0.54
2:B:14:LYS:NZ	2:B:234:SER:OG	2.38	0.54
2:B:673:ASP:OD1	2:B:677:LYS:N	2.38	0.54
1:A:702:ARG:NH2	2:B:427:ASP:OD2	2.41	0.54
1:A:85:LEU:HD11	1:A:95:ARG:HG2	1.90	0.53
1:A:833:LYS:NZ	2:B:1017:GLN:OE1	2.41	0.53
1:A:754:ALA:O	1:A:760:ARG:NH1	2.41	0.53
2:B:977:GLY:HA2	2:B:980:LEU:HD21	1.90	0.53
3:X:47:DA:H4'	3:X:48:DG:OP1	2.08	0.53
2:B:609:ALA:HB3	2:B:669:TYR:HB3	1.89	0.53
1:A:705:SER:HB2	1:A:758:LEU:HD13	1.90	0.53
2:B:72:ALA:HA	2:B:190:LEU:HD13	1.91	0.52
1:A:146:LEU:HD13	1:A:178:GLN:HB2	1.92	0.52
2:B:240:PRO:HB2	2:B:259:TYR:CD2	2.43	0.52
2:B:19:ILE:HG23	2:B:51:LEU:HD23	1.91	0.52
1:A:184:VAL:HG22	1:A:824:LEU:HD21	1.91	0.52
2:B:956:LEU:HD23	2:B:1002:THR:HB	1.90	0.52
2:B:284:HIS:CD2	2:B:290:LEU:HD12	2.44	0.51
1:A:497:GLY:H	1:A:501:GLY:HA3	1.73	0.51
2:B:983:LEU:HD13	2:B:1088:LEU:HB3	1.92	0.50
2:B:24:ASP:OD1	2:B:27:ARG:NH1	2.44	0.50
3:X:41:DC:H2"	3:X:42:DG:C8	2.46	0.50
1:A:268:ILE:HA	1:A:271:GLN:HG3	1.92	0.50
2:B:1107:ARG:NH2	2:B:1111:GLU:OE1	2.40	0.50
1:A:525:THR:HG23	1:A:878:LEU:HB3	1.93	0.50
2:B:1152:ILE:O	2:B:1156:ILE:HG13	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:386:PHE:CE1	2:B:412:LEU:HG	2.47	0.50
2:B:477:THR:HA	2:B:480:TRP:NE1	2.27	0.50
1:A:439:VAL:HG23	1:A:454:PHE:CD1	2.47	0.49
1:A:869:VAL:O	1:A:873:ARG:HG2	2.11	0.49
1:A:185:TYR:O	1:A:189:ARG:HG2	2.12	0.49
1:A:774:ASP:OD1	1:A:775:LEU:N	2.44	0.49
2:B:772:VAL:HG21	2:B:1110:ILE:HG13	1.95	0.49
2:B:495:ALA:HB1	2:B:500:GLU:HG3	1.94	0.49
1:A:32:ALA:O	1:A:477:ASN:ND2	2.44	0.49
2:B:222:GLU:O	2:B:226:VAL:HG23	2.12	0.49
1:A:137:GLU:CD	1:A:753:THR:HG23	2.33	0.48
1:A:1014:GLN:HG3	1:A:1152:LEU:HD13	1.95	0.48
2:B:770:ASN:H	2:B:1136:LEU:HD21	1.77	0.48
2:B:347:ILE:HG12	2:B:605:PHE:HB2	1.94	0.48
2:B:535:GLN:HG2	2:B:539:GLN:HE21	1.79	0.48
2:B:519:ASP:OD1	2:B:522:ARG:NH1	2.46	0.48
2:B:960:VAL:HG22	2:B:1007:LEU:HB2	1.95	0.48
1:A:756:ARG:H	1:A:756:ARG:HD2	1.78	0.48
2:B:287:THR:HG21	2:B:311:ALA:HB2	1.94	0.48
1:A:871:LEU:HG	1:A:878:LEU:HD21	1.96	0.47
1:A:818:LEU:HD21	1:A:855:MET:HB3	1.96	0.47
2:B:1055:LEU:HD22	2:B:1060:SER:HB2	1.96	0.47
1:A:107:SER:HB3	1:A:111:SER:HB3	1.97	0.47
1:A:589:LEU:HD11	1:A:598:ILE:HD12	1.96	0.47
1:A:1159:ASP:HB2	1:A:1172:ALA:HA	1.97	0.47
1:A:1018:GLU:O	1:A:1022:LYS:HG3	2.15	0.47
1:A:445:ARG:N	1:A:862:GLU:OE2	2.40	0.47
2:B:293:LEU:HD21	2:B:658:PHE:HB3	1.95	0.47
2:B:1115:MET:HB2	2:B:1144:LEU:HB2	1.96	0.47
1:A:124:ILE:HG13	1:A:374:TYR:HD1	1.80	0.47
1:A:522:GLU:O	1:A:877:LYS:NZ	2.40	0.47
1:A:1107:GLU:HA	1:A:1110:GLN:HB2	1.97	0.47
1:A:568:LYS:NZ	1:A:579:ASN:OD1	2.38	0.47
1:A:802:PRO:HB3	1:A:876:GLU:HG3	1.96	0.47
2:B:876:LEU:HA	2:B:882:HIS:HB3	1.96	0.46
1:A:67:ASN:ND2	3:X:57:DT:OP2	2.44	0.46
1:A:206:ASP:OD1	1:A:339:LYS:NZ	2.46	0.46
1:A:991:ASP:HA	2:B:745:SER:HB3	1.96	0.46
1:A:599:MET:HG2	1:A:609:VAL:HG11	1.97	0.46
3:X:46:DT:H2"	3:X:47:DA:C8	2.51	0.46
2:B:488:LEU:HD13	2:B:508:TYR:HB2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:971:LEU:HD22	2:B:1149:ASP:HB3	1.98	0.46
1:A:706:LYS:NZ	2:B:521:GLU:OE2	2.46	0.46
2:B:14:LYS:HG2	2:B:278:LEU:HD12	1.97	0.46
2:B:533:GLU:O	2:B:536:GLN:HG2	2.16	0.46
1:A:1195:LYS:HA	1:A:1198:GLU:HB2	1.97	0.46
3:X:55:DT:H1'	3:X:56:DT:H5'	1.98	0.45
3:X:7:DT:H2"	3:X:8:DC:C6	2.51	0.45
1:A:249:GLY:HA2	1:A:301:LEU:HD22	1.98	0.45
1:A:647:ARG:HH21	2:B:772:VAL:HG22	1.81	0.45
1:A:226:ILE:HG12	1:A:319:LEU:HD11	1.96	0.45
2:B:532:ILE:HD12	2:B:533:GLU:H	1.81	0.45
2:B:394:LEU:HG	2:B:489:GLN:HG3	1.98	0.45
1:A:57:VAL:HG23	1:A:97:GLN:OE1	2.16	0.45
2:B:532:ILE:HG13	2:B:532:ILE:H	1.51	0.45
2:B:21:SER:O	2:B:25:GLU:HG2	2.17	0.45
1:A:840:ARG:NH2	2:B:1015:MET:HG2	2.32	0.45
1:A:489:ASN:O	1:A:493:LYS:HB2	2.17	0.45
2:B:457:LEU:HD12	2:B:867:LEU:HD22	1.99	0.45
1:A:288:ARG:NH2	3:X:39:DC:O2	2.50	0.45
1:A:133:ALA:HB2	1:A:365:ILE:HG23	1.99	0.44
1:A:264:ILE:O	1:A:268:ILE:HG13	2.17	0.44
1:A:33:GLY:HA3	1:A:477:ASN:ND2	2.33	0.44
2:B:404:PHE:CZ	2:B:430:GLU:HA	2.53	0.44
1:A:551:GLU:OE1	1:A:883:SER:OG	2.34	0.44
1:A:861:SER:O	1:A:865:ARG:HG3	2.18	0.44
2:B:117:SER:O	2:B:120:THR:HG22	2.16	0.44
2:B:102:GLU:HG3	2:B:103:HIS:ND1	2.33	0.44
1:A:1002:TYR:OH	2:B:586:ASP:OD2	2.29	0.44
2:B:215:PRO:O	2:B:219:ARG:HG2	2.18	0.44
1:A:214:GLU:HA	1:A:219:TYR:CD2	2.53	0.44
2:B:398:TRP:HE1	2:B:489:GLN:NE2	2.16	0.44
2:B:992:HIS:O	2:B:996:TRP:HB3	2.17	0.44
1:A:103:ARG:HH21	2:B:643:GLY:HA3	1.83	0.44
2:B:283:ARG:HG3	2:B:662:SER:HA	1.99	0.44
2:B:330:GLU:OE2	2:B:698:ARG:NH1	2.50	0.44
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.82	0.43
2:B:299:ALA:O	2:B:687:ARG:NH2	2.43	0.43
1:A:495:LEU:HA	1:A:910:ARG:HD3	1.99	0.43
1:A:1049:PHE:CD1	2:B:552:VAL:HG21	2.53	0.43
2:B:986:LEU:HD21	2:B:1003:PRO:HB3	2.00	0.43
2:B:704:PRO:HG3	2:B:715:TYR:CE2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:47:DA:H1'	3:X:48:DG:O5'	2.18	0.43
2:B:822:GLU:HB3	2:B:824:PRO:HD2	2.00	0.43
2:B:747:TYR:O	2:B:751:MET:HG2	2.19	0.43
1:A:597:GLN:NE2	1:A:597:GLN:H	2.16	0.43
1:A:1086:VAL:HG12	1:A:1100:LYS:HD3	1.99	0.43
2:B:205:ILE:HG21	2:B:224:LEU:HD13	2.01	0.43
2:B:273:ILE:HG13	2:B:273:ILE:H	1.77	0.43
1:A:836:HIS:HA	1:A:837:PRO:HD3	1.81	0.43
2:B:39:VAL:HB	2:B:43:MET:HB3	2.01	0.43
1:A:595:ALA:HA	1:A:790:LEU:HD21	2.00	0.43
2:B:808:SER:HG	2:B:1126:PHE:HE2	1.67	0.43
1:A:41:VAL:O	1:A:45:ILE:HG12	2.18	0.42
1:A:1129:GLU:O	1:A:1131:PRO:HD3	2.19	0.42
2:B:895:ARG:NH1	2:B:1031:ILE:HG21	2.35	0.42
1:A:222:VAL:HG13	1:A:323:TYR:CE1	2.53	0.42
1:A:704:PHE:CD2	1:A:713:LEU:HD23	2.54	0.42
1:A:597:GLN:HE21	1:A:597:GLN:H	1.67	0.42
2:B:912:ILE:HB	2:B:946:VAL:HG23	2.02	0.42
2:B:237:ALA:HA	2:B:252:PHE:CD1	2.54	0.42
1:A:417:GLU:HG2	1:A:453:LEU:HD11	2.02	0.42
2:B:84:ARG:HD2	2:B:181:LEU:HB2	2.01	0.42
1:A:240:ALA:O	1:A:244:THR:HG23	2.20	0.42
2:B:515:PRO:HG3	2:B:541:TRP:CH2	2.55	0.42
3:X:37:DT:H2"	3:X:38:DG:C8	2.55	0.42
1:A:732:GLY:O	1:A:736:ARG:HG3	2.19	0.42
2:B:12:SER:HB2	2:B:278:LEU:HB3	2.01	0.42
1:A:458:TYR:OH	1:A:473:ASP:OD2	2.24	0.42
2:B:37:PHE:HB3	2:B:65:VAL:HA	2.02	0.42
1:A:479:ARG:NE	1:A:800:GLU:OE1	2.45	0.42
1:A:756:ARG:HH11	2:B:380:ASN:ND2	2.17	0.42
1:A:945:HIS:HA	1:A:946:PRO:HD3	1.83	0.42
2:B:128:THR:HG23	2:B:184:GLU:HG3	2.02	0.42
1:A:124:ILE:H	1:A:124:ILE:HD13	1.84	0.42
2:B:551:PHE:HE1	2:B:555:MET:HE3	1.85	0.42
1:A:85:LEU:HA	1:A:85:LEU:HD12	1.77	0.41
1:A:840:ARG:NH2	2:B:1013:ASP:O	2.53	0.41
2:B:88:THR:OG1	2:B:550:GLU:OE2	2.25	0.41
2:B:403:VAL:O	2:B:407:VAL:HG23	2.19	0.41
1:A:1201:ILE:HG13	1:A:1232:LEU:HD12	2.02	0.41
1:A:1141:ILE:HD12	1:A:1152:LEU:HD11	2.02	0.41
1:A:370:ASP:HB3	1:A:374:TYR:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:ASP:HB3	2:B:602:SER:HB2	2.03	0.41
2:B:9:ARG:HH22	2:B:298:GLU:HG2	1.86	0.41
1:A:1012:THR:OG1	2:B:584:ALA:O	2.38	0.41
1:A:338:MET:O	1:A:342:ILE:HG12	2.20	0.41
1:A:9:SER:O	1:A:10:THR:HG22	2.20	0.41
1:A:230:LEU:HD12	1:A:271:GLN:HE21	1.85	0.41
1:A:244:THR:HG21	1:A:254:ALA:HB2	2.01	0.41
1:A:727:VAL:HA	1:A:730:MET:HG2	2.02	0.41
1:A:170:THR:HG23	1:A:173:HIS:H	1.85	0.41
1:A:506:ASP:O	1:A:510:GLU:HG3	2.21	0.41
2:B:3:ALA:HB3	2:B:273:ILE:HG22	2.03	0.41
3:X:18:DC:H2"	3:X:19:DA:C8	2.56	0.41
2:B:971:LEU:HB3	2:B:1152:ILE:HG21	2.02	0.41
1:A:698:LEU:O	1:A:702:ARG:HG2	2.21	0.41
2:B:226:VAL:HG22	2:B:269:LEU:HD22	2.03	0.41
2:B:1005:GLY:HA2	2:B:1085:PHE:CZ	2.56	0.41
2:B:889:LEU:O	2:B:893:VAL:HG23	2.20	0.41
1:A:641:PRO:O	1:A:645:VAL:HG23	2.21	0.41
1:A:239:ARG:HA	1:A:239:ARG:HD3	1.85	0.41
2:B:1069:LYS:HE3	3:X:15:DG:H3'	2.02	0.41
1:A:897:SER:HB3	1:A:922:PRO:HB3	2.03	0.41
1:A:629:VAL:O	1:A:633:ILE:HG13	2.21	0.41
1:A:175:LEU:O	1:A:178:GLN:HG2	2.20	0.41
2:B:329:ARG:HD3	2:B:715:TYR:HA	2.03	0.41
2:B:287:THR:HA	2:B:288:PRO:HD3	1.74	0.40
1:A:166:ASP:HB3	1:A:837:PRO:HB3	2.03	0.40
1:A:750:TYR:OH	1:A:760:ARG:HB3	2.21	0.40
1:A:640:ILE:HB	1:A:641:PRO:HD3	2.02	0.40
3:X:14:DC:H2"	3:X:15:DG:C8	2.56	0.40
1:A:959:LEU:HA	1:A:959:LEU:HD12	1.89	0.40
1:A:894:TRP:CE2	1:A:921:GLY:HA3	2.57	0.40
2:B:1050:LEU:HA	2:B:1050:LEU:HD23	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	1136/1232 (92%)	1098 (97%)	38 (3%)	0	100	100
2	B	1142/1166 (98%)	1099 (96%)	41 (4%)	2 (0%)	52	87
All	All	2278/2398 (95%)	2197 (96%)	79 (4%)	2 (0%)	56	90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	13	GLY
2	B	998	GLY

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	1000/1062 (94%)	959 (96%)	41 (4%)	37	75
2	B	1015/1029 (99%)	973 (96%)	42 (4%)	37	75
All	All	2015/2091 (96%)	1932 (96%)	83 (4%)	37	75

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	65	PHE
1	A	84	GLU
1	A	124	ILE
1	A	146	LEU
1	A	237	LEU
1	A	326	ARG
1	A	400	GLN
1	A	422	LEU
1	A	448	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	458	TYR
1	A	459	LYS
1	A	500	ILE
1	A	508	GLN
1	A	531	ASP
1	A	546	GLU
1	A	551	GLU
1	A	594	TRP
1	A	597	GLN
1	A	622	GLU
1	A	672	GLU
1	A	685	ASP
1	A	706	LYS
1	A	746	ARG
1	A	756	ARG
1	A	770	GLU
1	A	806	VAL
1	A	816	MET
1	A	820	LYS
1	A	848	LEU
1	A	857	ARG
1	A	873	ARG
1	A	891	LEU
1	A	902	ASP
1	A	914	ARG
1	A	959	LEU
1	A	1064	MET
1	A	1068	MET
1	A	1100	LYS
1	A	1103	ILE
1	A	1230	LEU
2	B	37	PHE
2	B	41	ASP
2	B	56	ASP
2	B	60	MET
2	B	64	GLN
2	B	88	THR
2	B	97	ARG
2	B	125	ARG
2	B	169	TYR
2	B	218	PHE
2	B	265	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	284	HIS
2	B	287	THR
2	B	289	GLU
2	B	290	LEU
2	B	300	ARG
2	B	332	HIS
2	B	338	LYS
2	B	457	LEU
2	B	458	ASP
2	B	459	ASP
2	B	460	ASP
2	B	486	PHE
2	B	510	GLU
2	B	522	ARG
2	B	523	GLN
2	B	532	ILE
2	B	538	GLN
2	B	551	PHE
2	B	619	ASP
2	B	620	GLU
2	B	644	ARG
2	B	694	HIS
2	B	767	PHE
2	B	883	TYR
2	B	936	THR
2	B	999	MET
2	B	1063	ILE
2	B	1070	ASP
2	B	1085	PHE
2	B	1148	LYS
2	B	1149	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	135	GLN
1	A	220	GLN
1	A	269	GLN
1	A	271	GLN
1	A	577	HIS
1	A	597	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	794	HIS
1	A	836	HIS
1	A	912	GLN
1	A	1069	GLN
1	A	1113	HIS
2	B	227	HIS
2	B	270	ASN
2	B	292	HIS
2	B	316	GLN
2	B	351	GLN
2	B	463	GLN
2	B	489	GLN
2	B	535	GLN
2	B	758	GLN
2	B	817	GLN
2	B	1045	GLN
2	B	1131	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SF4	B	2161	2	0,12,12	0.00	-	0,24,24	0.00	-

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
4	SF4	B	2161	2	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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	1154/1232 (93%)	0.27	42 (3%)	46	34	64, 115, 170, 194	0
2	B	1148/1166 (98%)	0.31	55 (4%)	34	23	68, 123, 159, 185	1 (0%)
3	X	37/65 (56%)	1.34	13 (35%)	0	1	120, 191, 215, 222	0
All	All	2339/2463 (94%)	0.31	110 (4%)	35	24	64, 121, 168, 222	1 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	955	LEU	5.3
1	A	84	GLU	5.0
1	A	756	ARG	4.3
2	B	990	ILE	4.1
1	A	302	LEU	4.1
2	B	1066	GLY	4.1
1	A	252	PRO	4.0
1	A	1179	GLU	3.9
2	B	949	ALA	3.7
1	A	1178	ILE	3.7
2	B	603	CYS	3.6
2	B	706	GLN	3.6
2	B	5	PHE	3.5
2	B	1005	GLY	3.4
1	A	960	LEU	3.4
2	B	999	MET	3.3
2	B	237	ALA	3.3
1	A	927	HIS	3.3
1	A	1177	ARG	3.2
3	X	47	DA	3.2
2	B	168	LEU	3.1
3	X	49	DA	3.1
2	B	781	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	303	ILE	3.0
2	B	3	ALA	3.0
1	A	594	TRP	3.0
2	B	462	ALA	2.9
1	A	466	GLU	2.9
3	X	10	DA	2.9
1	A	290	LYS	2.9
1	A	528	LEU	2.8
1	A	297	PHE	2.8
3	X	39	DC	2.8
2	B	785	GLY	2.8
2	B	270	ASN	2.8
1	A	1169	TYR	2.8
1	A	553	LYS	2.8
1	A	1189	ALA	2.7
3	X	16	DA	2.7
2	B	659	SER	2.7
1	A	994	ALA	2.7
1	A	293	LYS	2.7
3	X	48	DG	2.7
1	A	292	VAL	2.7
3	X	37	DT	2.7
2	B	1069	LYS	2.7
2	B	178	ASP	2.6
1	A	1173	TYR	2.6
1	A	299	PRO	2.6
2	B	666	TYR	2.6
2	B	84	ARG	2.5
3	X	8	DC	2.5
3	X	50	DT	2.5
2	B	224	LEU	2.5
2	B	296	GLN	2.5
2	B	631	TRP	2.5
2	B	1000	ARG	2.5
2	B	1105	ASP	2.5
2	B	788	ILE	2.5
1	A	1223	PHE	2.5
1	A	585	ILE	2.4
2	B	109	VAL	2.4
1	A	1198	GLU	2.4
2	B	559	GLU	2.4
2	B	859	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	X	19	DA	2.4
1	A	1175	SER	2.4
2	B	699	LEU	2.4
2	B	897	SER	2.4
1	A	249	GLY	2.4
2	B	243	GLU	2.3
2	B	186	TYR	2.3
2	B	10	SER	2.3
1	A	303	ASP	2.3
1	A	776	GLY	2.3
2	B	777	ARG	2.3
2	B	15	THR	2.3
2	B	609	ALA	2.3
2	B	180	TYR	2.2
1	A	9	SER	2.2
1	A	1218	GLY	2.2
2	B	644	ARG	2.2
1	A	215	GLU	2.2
3	X	36	DG	2.2
2	B	1076	ASP	2.2
2	B	621	ASN	2.2
2	B	658	PHE	2.2
1	A	295	ASP	2.2
2	B	839	ASP	2.2
2	B	1059	ARG	2.2
2	B	83	SER	2.1
1	A	1079	ILE	2.1
2	B	555	MET	2.1
1	A	949	PHE	2.1
2	B	986	LEU	2.1
1	A	1021	ARG	2.1
2	B	1068	LYS	2.1
1	A	1228	HIS	2.1
2	B	344	ASP	2.1
1	A	1073	LEU	2.1
3	X	38	DG	2.1
2	B	1040	LEU	2.0
1	A	997	GLN	2.0
1	A	782	SER	2.0
1	A	1217	LYS	2.0
2	B	110	TYR	2.0
2	B	1003	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	786	ASP	2.0
3	X	52	DT	2.0
2	B	460	ASP	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
4	SF4	B	2161	8/8	0.99	0.21	-0.59	79,104,112,116	0

6.5 Other polymers (i)

There are no such residues in this entry.