Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:06 PM GMT

PDB ID	:	1NI4
Title	:	HUMAN PYRUVATE DEHYDROGENASE
Authors	:	Ciszak, E.; Korotchkina, L.G.; Dominiak, P.M.; Sidhu, S.; Patel, M.S.
Deposited on	:	2002-12-20
Resolution	:	1.95 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:

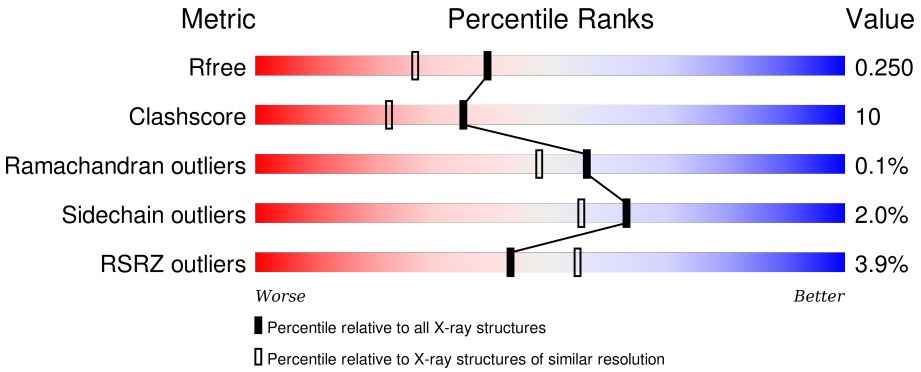
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	365	2% 79% 20%
1	C	365	5% 74% 24%
2	B	341	4% 77% 19%
2	D	341	4% 77% 19%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11496 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 Pyruvate dehydrogenase E1 component: Alpha subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	Se	0	0	0
			2824	1772	496	532	12	12			
1	C	362	Total	C	N	O	S	Se	0	0	0
			2824	1772	496	532	12	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	CLONING ARTIFACT	UNP P08559
A	-2	ARG	-	CLONING ARTIFACT	UNP P08559
A	-1	GLY	-	CLONING ARTIFACT	UNP P08559
A	0	SER	-	CLONING ARTIFACT	UNP P08559
A	38	MSE	MET	MODIFIED RESIDUE	UNP P08559
A	39	MSE	MET	MODIFIED RESIDUE	UNP P08559
A	45	MSE	MET	MODIFIED RESIDUE	UNP P08559
A	124	MSE	MET	MODIFIED RESIDUE	UNP P08559
A	126	MSE	MET	MODIFIED RESIDUE	UNP P08559
A	181	MSE	MET	MODIFIED RESIDUE	UNP P08559
A	200	MSE	MET	MODIFIED RESIDUE	UNP P08559
A	228	MSE	MET	MODIFIED RESIDUE	UNP P08559
A	253	MSE	MET	MODIFIED RESIDUE	UNP P08559
A	265	MSE	MET	MODIFIED RESIDUE	UNP P08559
A	289	MSE	MET	MODIFIED RESIDUE	UNP P08559
A	295	MSE	MET	MODIFIED RESIDUE	UNP P08559
C	-3	MET	-	CLONING ARTIFACT	UNP P08559
C	-2	ARG	-	CLONING ARTIFACT	UNP P08559
C	-1	GLY	-	CLONING ARTIFACT	UNP P08559
C	0	SER	-	CLONING ARTIFACT	UNP P08559
C	38	MSE	MET	MODIFIED RESIDUE	UNP P08559
C	39	MSE	MET	MODIFIED RESIDUE	UNP P08559
C	45	MSE	MET	MODIFIED RESIDUE	UNP P08559
C	124	MSE	MET	MODIFIED RESIDUE	UNP P08559
C	126	MSE	MET	MODIFIED RESIDUE	UNP P08559

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	181	MSE	MET	MODIFIED RESIDUE	UNP P08559
C	200	MSE	MET	MODIFIED RESIDUE	UNP P08559
C	228	MSE	MET	MODIFIED RESIDUE	UNP P08559
C	253	MSE	MET	MODIFIED RESIDUE	UNP P08559
C	265	MSE	MET	MODIFIED RESIDUE	UNP P08559
C	289	MSE	MET	MODIFIED RESIDUE	UNP P08559
C	295	MSE	MET	MODIFIED RESIDUE	UNP P08559

- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component: Beta subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	Se	0	0	0
			2525	1607	428	471	6	13			
2	D	330	Total	C	N	O	S	Se	0	0	0
			2525	1607	428	471	6	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	CLONING ARTIFACT	UNP P11177
B	-10	ARG	-	CLONING ARTIFACT	UNP P11177
B	-9	GLY	-	CLONING ARTIFACT	UNP P11177
B	-8	SER	-	CLONING ARTIFACT	UNP P11177
B	-7	HIS	-	EXPRESSION TAG	UNP P11177
B	-6	HIS	-	EXPRESSION TAG	UNP P11177
B	-5	HIS	-	EXPRESSION TAG	UNP P11177
B	-4	HIS	-	EXPRESSION TAG	UNP P11177
B	-3	HIS	-	EXPRESSION TAG	UNP P11177
B	-2	HIS	-	EXPRESSION TAG	UNP P11177
B	-1	GLY	-	CLONING ARTIFACT	UNP P11177
B	0	SER	-	CLONING ARTIFACT	UNP P11177
B	1	LEU	-	SEE REMARK 999	UNP P11177
B	13	MSE	MET	MODIFIED RESIDUE	UNP P11177
B	60	MSE	MET	MODIFIED RESIDUE	UNP P11177
B	71	MSE	MET	MODIFIED RESIDUE	UNP P11177
B	81	MSE	MET	MODIFIED RESIDUE	UNP P11177
B	87	MSE	MET	MODIFIED RESIDUE	UNP P11177
B	103	MSE	MET	MODIFIED RESIDUE	UNP P11177
B	175	MSE	MET	MODIFIED RESIDUE	UNP P11177
B	238	MSE	MET	MODIFIED RESIDUE	UNP P11177
B	244	MSE	MET	MODIFIED RESIDUE	UNP P11177
B	246	MSE	MET	MODIFIED RESIDUE	UNP P11177

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	254	MSE	MET	MODIFIED RESIDUE	UNP P11177
B	280	MSE	MET	MODIFIED RESIDUE	UNP P11177
B	302	MSE	MET	MODIFIED RESIDUE	UNP P11177
D	-11	MET	-	CLONING ARTIFACT	UNP P11177
D	-10	ARG	-	CLONING ARTIFACT	UNP P11177
D	-9	GLY	-	CLONING ARTIFACT	UNP P11177
D	-8	SER	-	CLONING ARTIFACT	UNP P11177
D	-7	HIS	-	EXPRESSION TAG	UNP P11177
D	-6	HIS	-	EXPRESSION TAG	UNP P11177
D	-5	HIS	-	EXPRESSION TAG	UNP P11177
D	-4	HIS	-	EXPRESSION TAG	UNP P11177
D	-3	HIS	-	EXPRESSION TAG	UNP P11177
D	-2	HIS	-	EXPRESSION TAG	UNP P11177
D	-1	GLY	-	CLONING ARTIFACT	UNP P11177
D	0	SER	-	CLONING ARTIFACT	UNP P11177
D	1	LEU	-	SEE REMARK 999	UNP P11177
D	13	MSE	MET	MODIFIED RESIDUE	UNP P11177
D	60	MSE	MET	MODIFIED RESIDUE	UNP P11177
D	71	MSE	MET	MODIFIED RESIDUE	UNP P11177
D	81	MSE	MET	MODIFIED RESIDUE	UNP P11177
D	87	MSE	MET	MODIFIED RESIDUE	UNP P11177
D	103	MSE	MET	MODIFIED RESIDUE	UNP P11177
D	175	MSE	MET	MODIFIED RESIDUE	UNP P11177
D	238	MSE	MET	MODIFIED RESIDUE	UNP P11177
D	244	MSE	MET	MODIFIED RESIDUE	UNP P11177
D	246	MSE	MET	MODIFIED RESIDUE	UNP P11177
D	254	MSE	MET	MODIFIED RESIDUE	UNP P11177
D	280	MSE	MET	MODIFIED RESIDUE	UNP P11177
D	302	MSE	MET	MODIFIED RESIDUE	UNP P11177

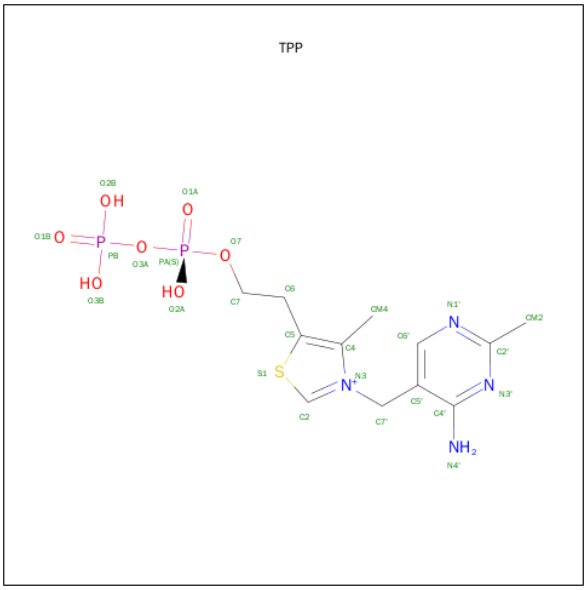
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O P S 26 12 4 7 2 1	0	0
5	A	1	Total C N O P S 26 12 4 7 2 1	0	0

- Molecule 6 is water.

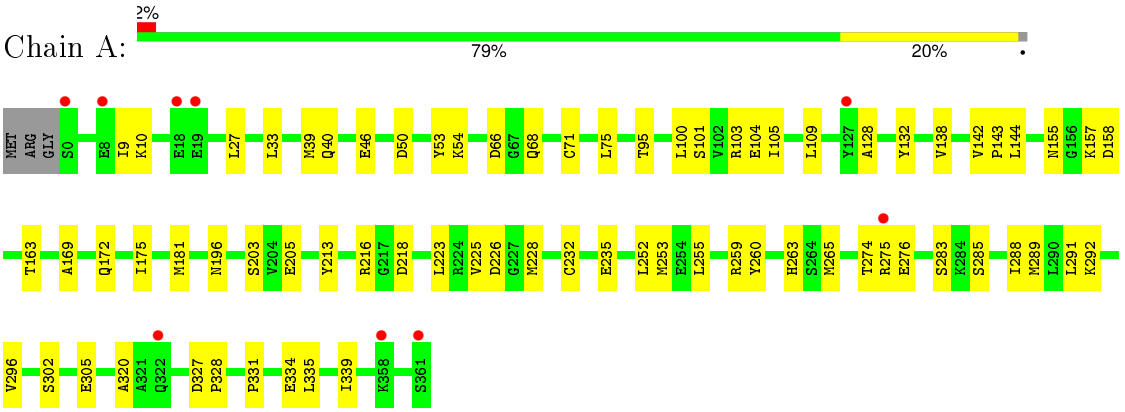
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	203	Total O 203 203	0	0
6	B	179	Total O 179 179	0	0
6	C	177	Total O 177 177	0	0
6	D	183	Total O 183 183	0	0

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.

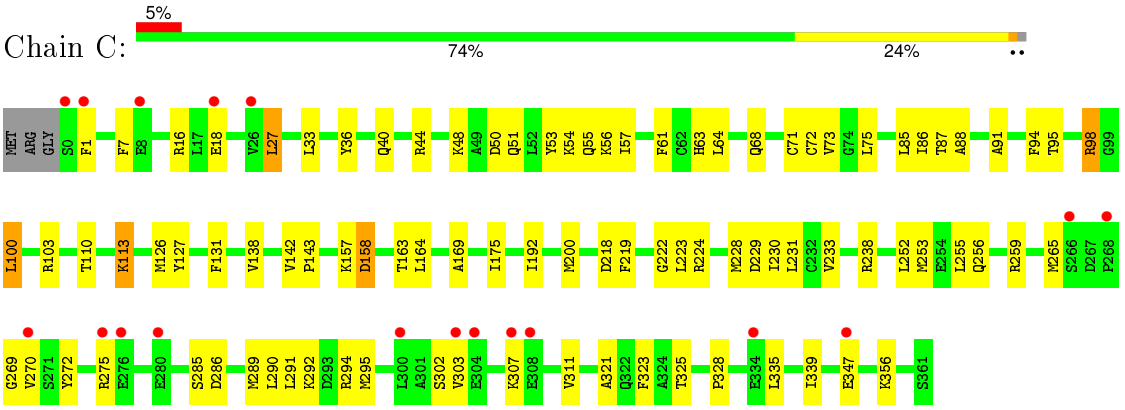
• Molecule 1: Pyruvate dehydrogenase E1 component: Alpha subunit

Chain A:



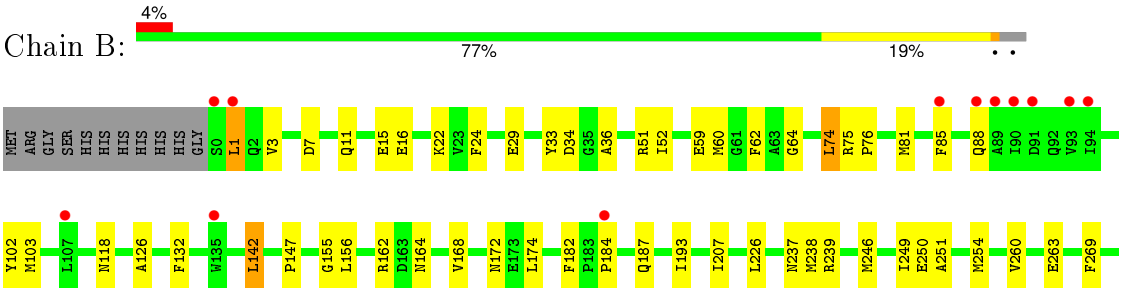
• Molecule 1: Pyruvate dehydrogenase E1 component: Alpha subunit

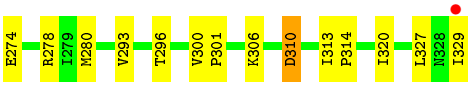
Chain C:



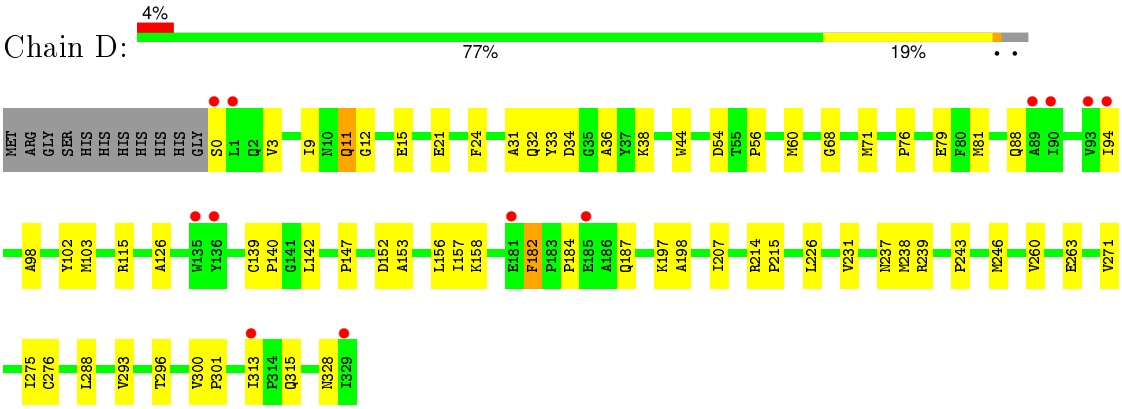
• Molecule 2: Pyruvate dehydrogenase E1 component: Beta subunit

Chain B:





• Molecule 2: Pyruvate dehydrogenase E1 component: Beta subunit



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.34Å 126.89Å 190.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.17 – 1.95 45.17 – 1.95	Depositor EDS
% Data completeness (in resolution range)	88.0 (45.17-1.95) 88.5 (45.17-1.95)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.244 0.220 , 0.250	Depositor DCC
R_{free} test set	9539 reflections (10.84%)	DCC
Wilson B-factor (Å^2)	12.6	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	3 of 188753 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	11496	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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: K, MG, TPP

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	0.32	0/2868	0.56	0/3842
1	C	0.32	0/2868	0.55	0/3842
2	B	0.33	0/2567	0.60	0/3457
2	D	0.33	0/2567	0.59	0/3457
All	All	0.32	0/10870	0.58	0/14598

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	2824	0	2780	59	0
1	C	2824	0	2780	67	0
2	B	2525	0	2522	47	0
2	D	2525	0	2522	52	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	26	0	16	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	26	0	16	0	0
6	A	203	0	0	4	0
6	B	179	0	0	5	0
6	C	177	0	0	4	0
6	D	183	0	0	4	0
All	All	11496	0	10636	210	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 10.

All (210) 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:29:GLU:HG3	1:C:200:MSE:HE2	1.41	1.01
1:C:98:ARG:HG2	1:C:131:PHE:HB2	1.47	0.92
2:D:12:GLY:HA3	2:D:157:ILE:HD11	1.53	0.91
1:C:291:LEU:HG	1:C:295:MSE:HE2	1.51	0.90
2:B:118:ASN:HD21	2:B:132:PHE:H	1.15	0.89
2:B:301:PRO:HG2	2:D:102:TYR:CD2	2.14	0.81
1:A:53:TYR:HB3	1:A:265:MSE:HE2	1.70	0.74
1:C:16:ARG:NH1	1:C:219:PHE:HA	2.02	0.73
1:C:95:THR:HG21	1:C:126:MSE:HE3	1.70	0.73
2:B:88:GLN:HG2	2:D:60:MSE:HE1	1.71	0.73
1:C:286:ASP:HB3	1:C:289:MSE:HG2	1.71	0.72
2:D:147:PRO:HB3	2:D:156:LEU:HD12	1.71	0.71
1:C:95:THR:HG22	1:C:131:PHE:CE2	2.26	0.71
2:B:251:ALA:HA	2:B:254:MSE:HE3	1.71	0.70
2:B:22:LYS:HE3	6:B:1420:HOH:O	1.93	0.69
1:A:339:ILE:HD11	2:D:300:VAL:HG12	1.73	0.68
2:B:300:VAL:HG12	1:C:339:ILE:HD11	1.77	0.66
1:C:71:CYS:O	1:C:75:LEU:HD13	1.96	0.65
2:D:260:VAL:HG22	2:D:293:VAL:HG22	1.78	0.65
2:B:75:ARG:HH22	2:B:164:ASN:ND2	1.94	0.65
2:B:102:TYR:CD2	2:D:301:PRO:HG2	2.32	0.65
2:D:98:ALA:HB2	2:D:142:LEU:HD13	1.79	0.64
2:B:75:ARG:HH22	2:B:164:ASN:HD22	1.45	0.64
2:B:118:ASN:HD21	2:B:132:PHE:N	1.94	0.63
1:A:103:ARG:NH1	1:A:320:ALA:HA	2.14	0.63
1:A:10:LYS:HG2	6:A:2460:HOH:O	1.99	0.62
1:C:50:ASP:OD1	1:C:54:LYS:HE3	2.00	0.62
2:B:22:LYS:HD2	2:B:74:LEU:HD12	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:HH11	1:A:320:ALA:HA	1.64	0.61
1:A:172:GLN:HB2	1:A:175:ILE:HD13	1.82	0.61
1:A:289:MSE:HE3	6:A:2474:HOH:O	2.00	0.61
1:C:292:LYS:HZ3	1:C:303:VAL:HG23	1.66	0.60
1:A:9:ILE:HB	1:A:232:CYS:SG	2.41	0.60
2:B:327:LEU:O	2:B:329:ILE:HG23	2.02	0.60
2:B:24:PHE:CZ	2:B:76:PRO:HB3	2.36	0.60
1:C:91:ALA:O	1:C:95:THR:HG23	2.02	0.59
1:A:142:VAL:HG21	1:A:175:ILE:HG13	1.84	0.59
1:A:283:SER:O	1:A:289:MSE:HE1	2.03	0.58
1:C:57:ILE:HG22	1:C:110:THR:HG22	1.84	0.58
2:D:0:SER:HB3	2:D:187:GLN:HE22	1.68	0.58
2:B:142:LEU:HD21	2:B:168:VAL:HG23	1.85	0.58
2:B:155:GLY:HA3	2:B:193:ILE:HG13	1.86	0.58
1:C:238:ARG:HD2	6:C:2477:HOH:O	2.03	0.58
1:A:172:GLN:HE22	2:D:88:GLN:HE22	1.51	0.58
6:B:1450:HOH:O	2:D:243:PRO:HA	2.04	0.58
1:A:50:ASP:OD1	1:A:265:MSE:HE1	2.04	0.57
2:B:260:VAL:HG22	2:B:293:VAL:HG22	1.86	0.57
2:B:313:ILE:HG23	2:B:314:PRO:HD2	1.87	0.57
1:A:253:MSE:HE3	1:A:255:LEU:HD11	1.85	0.57
2:D:33:TYR:O	2:D:34:ASP:HB2	2.05	0.57
1:A:68:GLN:HE21	1:A:259:ARG:HB3	1.68	0.57
1:C:7:PHE:CE2	1:C:294:ARG:HG2	2.40	0.57
2:D:207:ILE:HD11	2:D:260:VAL:HG23	1.86	0.56
1:C:335:LEU:O	1:C:335:LEU:HD23	2.05	0.56
2:D:246:MSE:HE1	2:D:275:ILE:HG23	1.85	0.56
1:A:181:MSE:HE1	2:B:62:PHE:N	2.20	0.56
2:D:139:CYS:HB3	6:D:2510:HOH:O	2.04	0.56
1:A:103:ARG:HG3	6:A:2386:HOH:O	2.05	0.56
1:A:68:GLN:HE22	1:A:196:ASN:HD22	1.53	0.55
1:A:142:VAL:HB	1:A:143:PRO:HD3	1.87	0.55
2:B:60:MSE:HE1	2:D:88:GLN:HG2	1.87	0.55
1:A:144:LEU:HD23	2:B:64:GLY:O	2.07	0.55
1:A:95:THR:CG2	1:A:100:LEU:HD22	2.37	0.55
1:A:142:VAL:HA	1:A:163:THR:HG21	1.87	0.54
1:C:292:LYS:NZ	1:C:303:VAL:HG23	2.22	0.54
1:C:229:ASP:CG	1:C:294:ARG:HH12	2.10	0.54
2:D:79:GLU:CD	2:D:115:ARG:HH12	2.11	0.54
2:D:12:GLY:HA3	2:D:157:ILE:CD1	2.34	0.54
1:A:335:LEU:HD23	1:A:335:LEU:C	2.28	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:TYR:HB3	1:C:265:MSE:HE2	1.90	0.54
1:A:103:ARG:HG2	1:A:103:ARG:HH11	1.73	0.54
1:C:222:GLY:HA2	1:C:252:LEU:O	2.08	0.54
1:C:55:GLN:O	1:C:56:LYS:HB2	2.06	0.54
2:B:246:MSE:HE3	2:B:249:ILE:HB	1.90	0.54
2:B:36:ALA:HB2	2:B:81:MSE:HE2	1.90	0.54
2:B:260:VAL:HG22	2:B:293:VAL:CG2	2.38	0.53
1:C:142:VAL:HA	1:C:163:THR:HG21	1.90	0.53
1:A:327:ASP:OD1	1:A:328:PRO:HD2	2.08	0.53
2:B:207:ILE:HD11	2:B:260:VAL:HG23	1.90	0.53
1:C:95:THR:HG22	1:C:131:PHE:HE2	1.70	0.53
2:B:118:ASN:ND2	2:B:132:PHE:H	1.96	0.52
1:A:205:GLU:H	1:A:205:GLU:CD	2.13	0.52
1:C:103:ARG:HG2	1:C:323:PHE:CD2	2.44	0.52
1:A:302:SER:OG	1:A:305:GLU:HG3	2.09	0.52
1:C:75:LEU:HD11	1:C:255:LEU:HD21	1.91	0.52
2:D:94:ILE:HD12	2:D:139:CYS:SG	2.50	0.52
2:B:11:GLN:O	2:B:15:GLU:HG3	2.10	0.52
1:C:113:LYS:NZ	1:C:113:LYS:HB2	2.26	0.51
2:D:34:ASP:O	2:D:38:LYS:HA	2.11	0.51
2:D:0:SER:HB3	2:D:187:GLN:NE2	2.26	0.51
2:D:24:PHE:CZ	2:D:76:PRO:HB3	2.45	0.51
2:D:313:ILE:HG23	2:D:315:GLN:HE21	1.76	0.51
1:C:87:THR:HG21	1:C:91:ALA:HB2	1.92	0.50
1:C:113:LYS:HD3	1:C:328:PRO:HG2	1.92	0.50
1:A:213:TYR:HA	1:A:216:ARG:HG2	1.93	0.50
1:C:73:VAL:HG12	1:C:230:ILE:HD11	1.92	0.50
1:A:331:PRO:HG2	1:A:334:GLU:HG3	1.93	0.50
6:B:1456:HOH:O	2:D:60:MSE:HE2	2.12	0.49
2:D:313:ILE:HG23	2:D:315:GLN:NE2	2.27	0.49
1:A:68:GLN:NE2	1:A:259:ARG:HB3	2.26	0.49
1:A:274:THR:OG1	1:A:276:GLU:HG3	2.12	0.49
1:C:228:MSE:HE3	1:C:285:SER:O	2.13	0.49
2:B:250:GLU:O	2:B:254:MSE:HG3	2.12	0.48
2:D:21:GLU:HG2	6:D:2490:HOH:O	2.12	0.48
2:D:31:ALA:HB3	2:D:54:ASP:OD2	2.13	0.48
1:C:253:MSE:HE3	1:C:255:LEU:HD11	1.96	0.48
1:C:270:VAL:O	1:C:270:VAL:HG22	2.13	0.48
1:A:235:GLU:HG2	6:A:2407:HOH:O	2.13	0.48
2:D:11:GLN:O	2:D:15:GLU:HG3	2.12	0.48
1:C:289:MSE:HG3	1:C:290:LEU:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:HA	1:A:163:THR:CG2	2.44	0.48
1:A:203:SER:HB2	1:A:205:GLU:OE2	2.13	0.48
1:A:223:LEU:HD23	1:A:252:LEU:O	2.14	0.48
2:B:16:GLU:OE1	2:B:162:ARG:HD2	2.13	0.48
2:B:184:PRO:HA	2:B:187:GLN:NE2	2.29	0.47
2:B:238:MSE:O	2:B:239:ARG:HB2	2.13	0.47
2:D:68:GLY:HA2	2:D:71:MSE:HE2	1.95	0.47
2:D:313:ILE:HD12	6:D:2485:HOH:O	2.13	0.47
2:B:269:PHE:HE1	2:D:271:VAL:HA	1.80	0.47
1:C:335:LEU:C	1:C:335:LEU:HD23	2.35	0.47
2:D:238:MSE:O	2:D:239:ARG:HB2	2.13	0.47
1:C:87:THR:CG2	1:C:91:ALA:HB2	2.45	0.47
1:C:224:ARG:HD2	1:C:256:GLN:NE2	2.30	0.47
1:A:138:VAL:HG13	1:A:169:ALA:HB2	1.97	0.46
2:B:1:LEU:HD12	2:B:3:VAL:CG1	2.45	0.46
2:B:147:PRO:HB3	2:B:156:LEU:HD12	1.96	0.46
1:C:68:GLN:HE21	1:C:259:ARG:HB3	1.80	0.46
1:A:100:LEU:HD13	1:A:128:ALA:HB2	1.98	0.46
1:C:356:LYS:N	1:C:356:LYS:HD2	2.31	0.46
1:A:9:ILE:CD1	1:A:235:GLU:HG3	2.46	0.46
1:A:68:GLN:NE2	1:A:196:ASN:HD22	2.13	0.46
2:D:79:GLU:HG3	2:D:115:ARG:NH1	2.31	0.46
1:C:1:PHE:HZ	1:C:302:SER:HB3	1.81	0.46
2:D:152:ASP:OD1	2:D:239:ARG:NE	2.47	0.45
1:A:95:THR:HG22	1:A:100:LEU:HB2	1.98	0.45
2:B:33:TYR:O	2:B:34:ASP:HB2	2.16	0.45
1:A:95:THR:HG23	1:A:100:LEU:HD22	1.99	0.45
1:C:142:VAL:HB	1:C:143:PRO:HD3	1.98	0.45
2:B:280:MSE:CE	2:D:276:CYS:HB3	2.46	0.45
1:C:321:ALA:O	1:C:325:THR:HG23	2.16	0.45
2:D:0:SER:HB2	2:D:184:PRO:HD3	1.99	0.45
1:C:91:ALA:HA	6:C:2379:HOH:O	2.17	0.44
2:B:51:ARG:O	2:B:52:ILE:HD13	2.17	0.44
2:B:22:LYS:HG3	6:B:1500:HOH:O	2.16	0.44
2:B:274:GLU:O	2:B:278:ARG:HG2	2.17	0.44
1:A:39:MSE:CE	1:A:291:LEU:HD22	2.47	0.44
6:B:1439:HOH:O	2:D:88:GLN:HG3	2.17	0.44
1:C:40:GLN:O	1:C:44:ARG:HG2	2.18	0.44
1:A:225:VAL:HG12	1:A:226:ASP:N	2.33	0.44
1:A:132:TYR:N	1:A:132:TYR:CD1	2.86	0.44
2:B:306:LYS:HD3	2:B:310:ASP:OD1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:157:ILE:HG13	2:D:158:LYS:N	2.33	0.43
1:C:53:TYR:CG	1:C:265:MSE:HG3	2.52	0.43
2:B:263:GLU:HG2	2:B:296:THR:HG22	2.00	0.43
1:C:127:TYR:N	1:C:127:TYR:CD1	2.86	0.43
2:D:56:PRO:HA	6:D:2455:HOH:O	2.18	0.43
2:D:153:ALA:O	2:D:157:ILE:HG23	2.18	0.43
1:A:39:MSE:HE1	1:A:291:LEU:HD22	2.00	0.43
1:A:105:ILE:O	1:A:109:LEU:HD13	2.18	0.43
1:A:50:ASP:OD2	1:A:54:LYS:NZ	2.51	0.43
2:B:103:MSE:SE	2:D:126:ALA:HB3	2.68	0.43
2:B:226:LEU:HD21	2:B:320:ILE:HG23	2.00	0.43
1:C:61:PHE:HB3	1:C:63:HIS:CE1	2.53	0.43
1:C:138:VAL:HG13	1:C:169:ALA:HB2	2.00	0.43
1:C:94:PHE:O	1:C:98:ARG:HB2	2.19	0.43
2:D:9:ILE:HA	2:D:157:ILE:HD13	2.00	0.43
1:C:270:VAL:HG21	1:C:275:ARG:NH1	2.34	0.43
1:C:269:GLY:HA2	1:C:272:TYR:CE1	2.54	0.43
1:C:100:LEU:HA	1:C:100:LEU:HD12	1.89	0.43
2:D:226:LEU:HB3	2:D:231:VAL:HB	2.01	0.43
2:B:172:ASN:HD21	2:B:174:LEU:HB2	1.82	0.43
1:C:36:TYR:HB2	1:C:295:MSE:HE1	2.01	0.43
1:A:71:CYS:SG	1:A:255:LEU:HD23	2.59	0.43
2:D:139:CYS:HA	2:D:140:PRO:HD3	1.82	0.42
1:C:307:LYS:O	1:C:311:VAL:HG23	2.19	0.42
1:A:66:ASP:OD1	1:A:260:TYR:HB2	2.18	0.42
2:D:214:ARG:N	2:D:215:PRO:HD2	2.34	0.42
1:A:275:ARG:HH11	1:A:275:ARG:HG2	1.84	0.42
2:D:197:LYS:HD2	2:D:198:ALA:O	2.19	0.42
2:D:197:LYS:HD3	2:D:198:ALA:N	2.35	0.42
1:C:85:LEU:HD23	1:C:86:ILE:N	2.35	0.42
1:C:157:LYS:O	1:C:158:ASP:HB2	2.19	0.42
1:A:100:LEU:HD13	1:A:128:ALA:CB	2.49	0.42
1:A:172:GLN:CB	1:A:175:ILE:HD13	2.50	0.41
1:A:101:SER:OG	1:A:104:GLU:HG3	2.19	0.41
1:A:263:HIS:CE1	5:A:2330:TPP:S1	3.13	0.41
1:C:103:ARG:NH1	6:C:2506:HOH:O	2.52	0.41
1:C:53:TYR:CD2	1:C:265:MSE:HG3	2.55	0.41
1:C:27:LEU:HG	1:C:231:LEU:HD21	2.02	0.41
1:C:48:LYS:NZ	1:C:51:GLN:NE2	2.68	0.41
2:B:126:ALA:HB3	2:D:103:MSE:SE	2.71	0.41
2:D:36:ALA:HB2	2:D:81:MSE:HE2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:GLU:HG2	2:B:85:PHE:O	2.21	0.41
1:C:88:ALA:HB3	6:C:2356:HOH:O	2.21	0.41
1:C:72:CYS:HA	1:C:94:PHE:CE1	2.54	0.41
1:A:157:LYS:O	1:A:158:ASP:HB3	2.20	0.41
1:C:223:LEU:HD23	1:C:223:LEU:N	2.35	0.41
1:C:142:VAL:HG21	1:C:175:ILE:HG12	2.02	0.41
1:A:292:LYS:O	1:A:296:VAL:HG23	2.21	0.41
1:C:64:LEU:HD22	1:C:64:LEU:N	2.36	0.41
2:D:32:GLN:HG2	2:D:44:TRP:CH2	2.56	0.41
1:A:228:MSE:HE3	1:A:285:SER:O	2.21	0.41
1:C:75:LEU:HD12	1:C:233:VAL:CG1	2.51	0.40
2:D:3:VAL:HG21	2:D:182:PHE:CG	2.56	0.40
2:D:263:GLU:HG2	2:D:296:THR:HG22	2.03	0.40
1:C:259:ARG:O	1:C:259:ARG:HG3	2.21	0.40
1:C:164:LEU:HG	1:C:192:ILE:HB	2.04	0.40
1:A:155:ASN:OD1	2:B:22:LYS:HE2	2.21	0.40
1:A:46:GLU:HA	1:A:46:GLU:OE1	2.21	0.40
1:A:40:GLN:HE21	1:A:288:ILE:HD13	1.86	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	360/365 (99%)	349 (97%)	10 (3%)	1 (0%)	46	35
1	C	360/365 (99%)	349 (97%)	10 (3%)	1 (0%)	46	35
2	B	328/341 (96%)	316 (96%)	12 (4%)	0	100	100
2	D	328/341 (96%)	317 (97%)	11 (3%)	0	100	100
All	All	1376/1412 (98%)	1331 (97%)	43 (3%)	2 (0%)	56	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	218	ASP
1	A	218	ASP

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	295/285 (104%)	292 (99%)	3 (1%)	82	80
1	C	295/285 (104%)	287 (97%)	8 (3%)	52	41
2	B	269/265 (102%)	262 (97%)	7 (3%)	54	43
2	D	269/265 (102%)	264 (98%)	5 (2%)	65	58
All	All	1128/1100 (102%)	1105 (98%)	23 (2%)	63	55

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	33	LEU
1	A	75	LEU
2	B	1	LEU
2	B	7	ASP
2	B	74	LEU
2	B	142	LEU
2	B	182	PHE
2	B	237	ASN
2	B	310	ASP
1	C	18	GLU
1	C	27	LEU
1	C	33	LEU
1	C	98	ARG
1	C	100	LEU
1	C	113	LYS
1	C	158	ASP
1	C	347	GLU
2	D	11	GLN
2	D	182	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	237	ASN
2	D	288	LEU
2	D	328	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	40	GLN
1	A	55	GLN
1	A	68	GLN
1	A	80	ASN
1	A	130	ASN
1	A	297	ASN
2	B	32	GLN
2	B	88	GLN
2	B	118	ASN
2	B	164	ASN
2	B	172	ASN
2	B	187	GLN
2	B	237	ASN
2	B	257	ASN
1	C	3	ASN
1	C	40	GLN
1	C	51	GLN
1	C	55	GLN
1	C	68	GLN
1	C	80	ASN
1	C	256	GLN
1	C	299	ASN
2	D	88	GLN
2	D	187	GLN
2	D	237	ASN
2	D	315	GLN
2	D	328	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
5	TPP	A	2330	3	20,27,27	2.41	2 (10%)	31,40,40	1.65	4 (12%)
5	TPP	C	1330	3	20,27,27	2.61	2 (10%)	31,40,40	1.62	4 (12%)

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
5	TPP	A	2330	3	-	0/16/17/17	0/2/2/2
5	TPP	C	1330	3	-	0/16/17/17	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1330	TPP	CM4-C4	2.14	1.54	1.49
5	A	2330	TPP	CM4-C4	2.17	1.54	1.49
5	A	2330	TPP	C4-N3	9.46	1.47	1.39
5	C	1330	TPP	C4-N3	10.60	1.48	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2330	TPP	C6-C5-S1	-4.76	113.58	120.24
5	C	1330	TPP	C6-C5-S1	-4.66	113.72	120.24
5	C	1330	TPP	O3A-PA-O7	2.95	110.77	102.94
5	C	1330	TPP	C6'-N1'-C2'	3.01	121.03	115.77
5	A	2330	TPP	C6'-N1'-C2'	3.09	121.16	115.77
5	A	2330	TPP	O3A-PA-O7	3.20	111.43	102.94
5	A	2330	TPP	C6-C5-C4	3.47	130.67	127.56
5	C	1330	TPP	C6-C5-C4	3.63	130.81	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2330	TPP	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	350/365 (95%)	0.57	9 (2%) 59 69	5, 17, 30, 42	0
1	C	350/365 (95%)	0.74	18 (5%) 32 43	5, 19, 40, 50	0
2	B	317/341 (92%)	0.55	13 (4%) 41 52	5, 14, 27, 49	0
2	D	317/341 (92%)	0.53	12 (3%) 44 56	5, 14, 27, 37	0
All	All	1334/1412 (94%)	0.60	52 (3%) 43 54	5, 16, 33, 50	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	0	SER	5.1
1	C	270	VAL	4.5
1	A	18	GLU	4.1
2	B	329	ILE	4.0
2	D	181	GLU	3.9
2	D	1	LEU	3.7
1	C	275	ARG	3.5
2	D	329	ILE	3.3
2	D	90	ILE	3.3
2	B	1	LEU	3.2
1	C	0	SER	3.0
2	D	94	ILE	2.9
2	B	89	ALA	2.9
2	B	94	ILE	2.9
2	D	89	ALA	2.9
1	C	280	GLU	2.9
1	C	303	VAL	2.9
1	A	361	SER	2.8
2	B	90	ILE	2.7
2	D	93	VAL	2.7
1	C	18	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	184	PRO	2.7
1	C	276	GLU	2.6
1	A	275	ARG	2.6
1	C	26	VAL	2.6
1	A	0	SER	2.6
1	A	8	GLU	2.6
1	C	266	SER	2.6
1	C	304	GLU	2.5
1	A	19	GLU	2.5
1	C	300	LEU	2.5
2	B	93	VAL	2.4
1	C	1	PHE	2.4
2	B	135	TRP	2.4
2	D	313	ILE	2.4
2	D	185	GLU	2.4
2	D	0	SER	2.3
2	B	91	ASP	2.3
1	C	8	GLU	2.3
1	A	358	LYS	2.3
2	B	88	GLN	2.3
1	C	308	GLU	2.3
1	A	127	TYR	2.2
1	C	347	GLU	2.2
1	C	334	GLU	2.2
2	D	135	TRP	2.1
1	A	322	GLN	2.1
2	D	136	TYR	2.1
2	B	107	LEU	2.1
1	C	268	PRO	2.1
1	C	307	LYS	2.0
2	B	85	PHE	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

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
3	MG	C	2331	1/1	0.98	0.17	1.22	5,5,5,5	0
5	TPP	C	1330	26/26	0.95	0.14	-0.27	8,19,25,27	0
5	TPP	A	2330	26/26	0.96	0.13	-0.36	6,16,22,24	0
3	MG	A	1331	1/1	0.98	0.12	-0.54	5,5,5,5	0
4	K	B	1332	1/1	0.99	0.06	-4.08	12,12,12,12	0
4	K	D	2332	1/1	0.99	0.04	-4.65	12,12,12,12	0

6.5 Other polymers

There are no such residues in this entry.