Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2024 – 09:30 PM EDT

PDB ID	:	2BBD
Title	:	Crystal Structure of the STIV MCP
Authors	:	Khayat, R.
Deposited on	:	2005-10-17
Resolution	:	2.04 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:

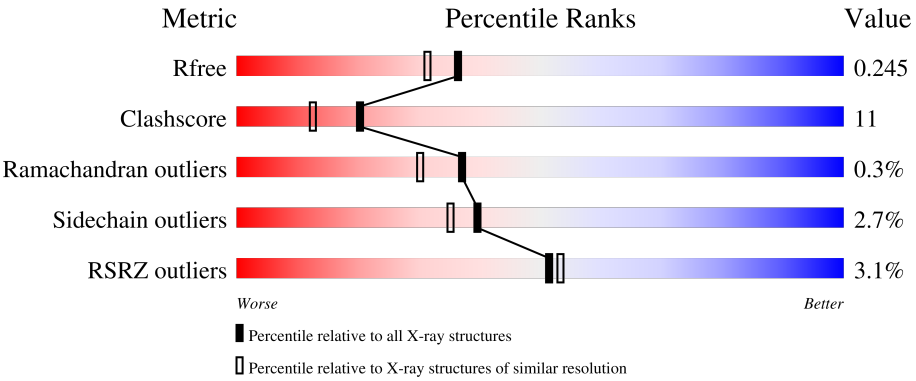
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.04 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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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	350	2% 77% 15% 8%
1	B	350	3% 71% 20% • 8%
1	C	350	4% 67% 24% • 8%
1	D	350	2% 74% 17% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10870 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 coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	Se	0	0	0
			2488	1600	400	484	4			
1	B	323	Total	C	N	O	Se	0	0	0
			2491	1603	400	484	4			
1	C	323	Total	C	N	O	Se	0	0	0
			2488	1600	400	484	4			
1	D	323	Total	C	N	O	Se	0	0	0
			2488	1600	400	484	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	MSE	MET	modified residue	UNP Q6Q0J0
A	116	MSE	MET	modified residue	UNP Q6Q0J0
A	128	MSE	MET	modified residue	UNP Q6Q0J0
A	177	MSE	MET	modified residue	UNP Q6Q0J0
A	346	HIS	-	expression tag	UNP Q6Q0J0
A	347	HIS	-	expression tag	UNP Q6Q0J0
A	348	HIS	-	expression tag	UNP Q6Q0J0
A	349	HIS	-	expression tag	UNP Q6Q0J0
A	350	HIS	-	expression tag	UNP Q6Q0J0
A	351	HIS	-	expression tag	UNP Q6Q0J0
B	87	MSE	MET	modified residue	UNP Q6Q0J0
B	116	MSE	MET	modified residue	UNP Q6Q0J0
B	128	MSE	MET	modified residue	UNP Q6Q0J0
B	177	MSE	MET	modified residue	UNP Q6Q0J0
B	346	HIS	-	expression tag	UNP Q6Q0J0
B	347	HIS	-	expression tag	UNP Q6Q0J0
B	348	HIS	-	expression tag	UNP Q6Q0J0
B	349	HIS	-	expression tag	UNP Q6Q0J0
B	350	HIS	-	expression tag	UNP Q6Q0J0
B	351	HIS	-	expression tag	UNP Q6Q0J0
C	87	MSE	MET	modified residue	UNP Q6Q0J0

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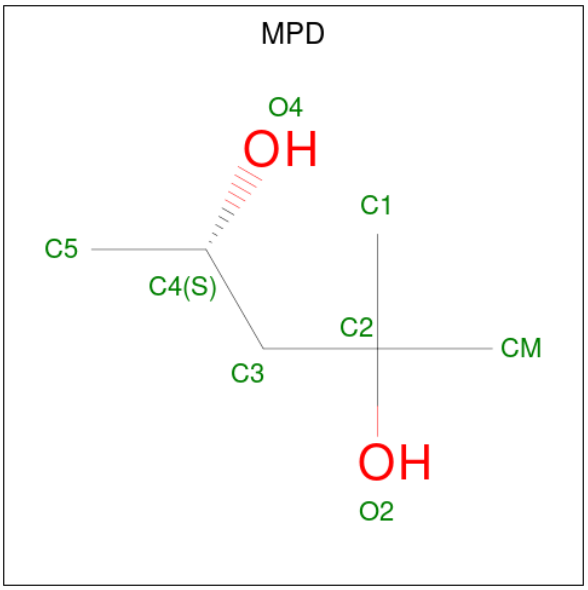
Chain	Residue	Modelled	Actual	Comment	Reference
C	116	MSE	MET	modified residue	UNP Q6Q0J0
C	128	MSE	MET	modified residue	UNP Q6Q0J0
C	177	MSE	MET	modified residue	UNP Q6Q0J0
C	346	HIS	-	expression tag	UNP Q6Q0J0
C	347	HIS	-	expression tag	UNP Q6Q0J0
C	348	HIS	-	expression tag	UNP Q6Q0J0
C	349	HIS	-	expression tag	UNP Q6Q0J0
C	350	HIS	-	expression tag	UNP Q6Q0J0
C	351	HIS	-	expression tag	UNP Q6Q0J0
D	87	MSE	MET	modified residue	UNP Q6Q0J0
D	116	MSE	MET	modified residue	UNP Q6Q0J0
D	128	MSE	MET	modified residue	UNP Q6Q0J0
D	177	MSE	MET	modified residue	UNP Q6Q0J0
D	346	HIS	-	expression tag	UNP Q6Q0J0
D	347	HIS	-	expression tag	UNP Q6Q0J0
D	348	HIS	-	expression tag	UNP Q6Q0J0
D	349	HIS	-	expression tag	UNP Q6Q0J0
D	350	HIS	-	expression tag	UNP Q6Q0J0
D	351	HIS	-	expression tag	UNP Q6Q0J0

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	B	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	254	Total O 254 254	0	0
3	B	143	Total O 143 143	0	0
3	C	143	Total O 143 143	0	0

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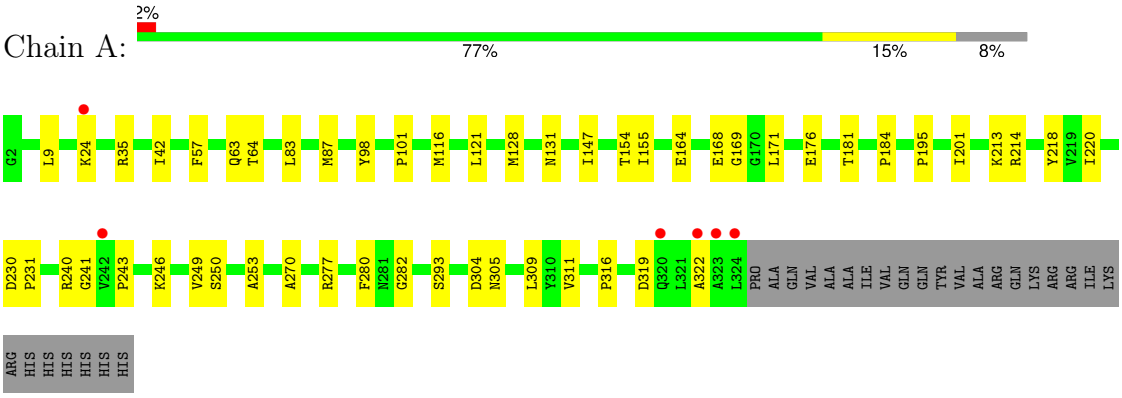
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	239	Total O 239 239	0	0

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.

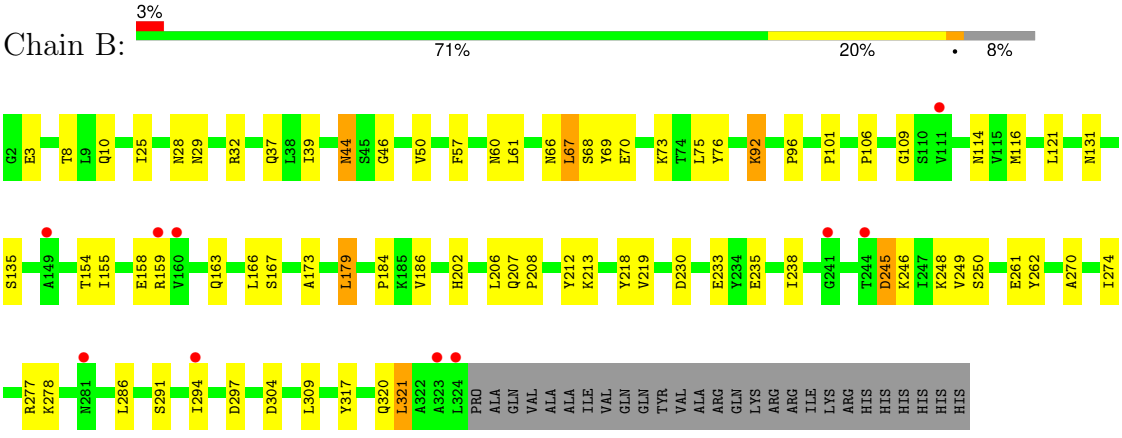
• Molecule 1: coat protein

Chain A:



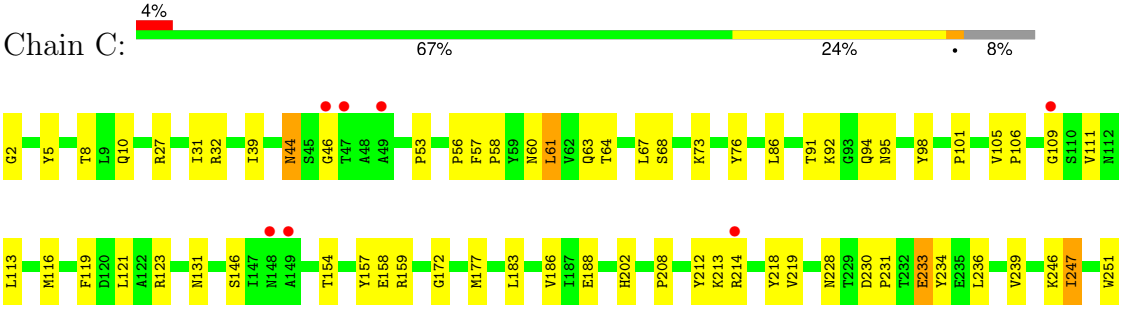
• Molecule 1: coat protein

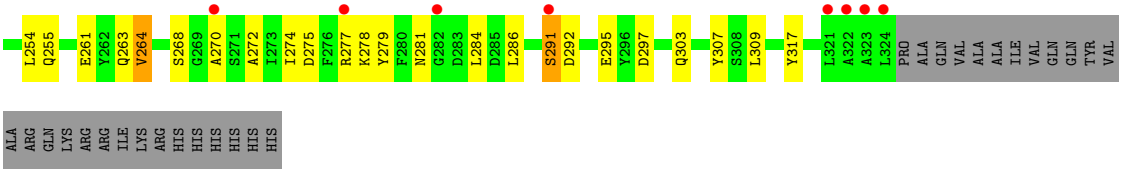
Chain B:



• Molecule 1: coat protein

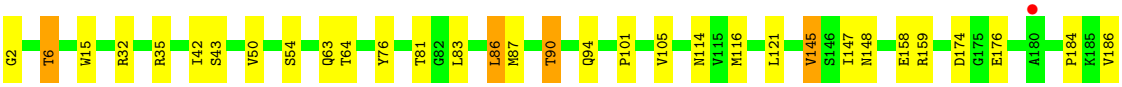
Chain C:

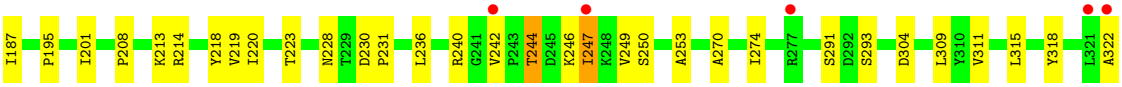


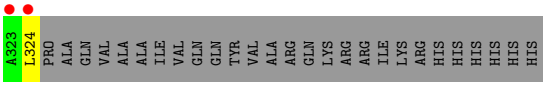


• Molecule 1: coat protein

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	241.60Å 82.89Å 114.80Å 90.00° 116.00° 90.00°	Depositor
Resolution (Å)	29.76 – 2.04 29.76 – 2.04	Depositor EDS
% Data completeness (in resolution range)	76.4 (29.76-2.04) 80.7 (29.76-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.246 0.207 , 0.245	Depositor DCC
R_{free} test set	7769 reflections (7.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10870	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: MPD

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	0.37	0/2545	0.65	0/3480
1	B	0.33	0/2548	0.63	0/3484
1	C	0.33	0/2545	0.62	0/3480
1	D	0.36	0/2545	0.64	0/3480
All	All	0.35	0/10183	0.64	0/13924

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	2488	0	2457	43	0
1	B	2491	0	2466	59	0
1	C	2488	0	2457	76	0
1	D	2488	0	2457	44	0
2	A	64	0	112	6	0
2	B	8	0	14	0	0
2	C	40	0	70	8	0
2	D	24	0	42	3	0
3	A	254	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	143	0	0	6	0
3	C	143	0	0	4	0
3	D	239	0	0	2	0
All	All	10870	0	10075	224	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 11.

All (224) 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:C:236:LEU:HB3	1:C:247:ILE:HG23	1.41	1.03
1:C:228:ASN:HD22	1:C:230:ASP:H	1.13	0.97
1:D:228:ASN:HD22	1:D:230:ASP:H	1.21	0.89
1:A:240:ARG:HH11	1:A:240:ARG:HB2	1.35	0.88
1:C:208:PRO:HG2	1:C:291:SER:HA	1.55	0.88
1:A:305:ASN:HD21	2:A:1005:MPD:H53	1.42	0.84
1:D:236:LEU:HB3	1:D:247:ILE:HG23	1.59	0.83
1:D:240:ARG:HG3	1:D:293:SER:HA	1.64	0.80
1:C:254:LEU:HD22	1:C:272:ALA:HB1	1.63	0.78
1:B:44:ASN:ND2	1:B:46:GLY:H	1.82	0.78
1:B:261:GLU:HG3	1:B:278:LYS:NZ	1.99	0.77
3:A:1148:HOH:O	1:D:6:THR:HG23	1.86	0.75
1:A:24:LYS:HE3	1:A:131:ASN:HA	1.70	0.73
1:C:236:LEU:HB3	1:C:247:ILE:CG2	2.17	0.72
1:D:219:VAL:HG22	1:D:270:ALA:HB1	1.71	0.72
1:C:292:ASP:N	3:C:1156:HOH:O	2.22	0.72
1:C:32:ARG:HD3	1:C:158:GLU:OE2	1.93	0.69
1:D:86:LEU:O	1:D:90:THR:HB	1.92	0.68
1:D:213:LYS:HE3	1:D:214:ARG:NH1	2.08	0.68
1:A:240:ARG:HB2	1:A:240:ARG:NH1	2.08	0.67
1:C:8:THR:OG1	1:C:154:THR:HG22	1.94	0.67
1:A:277:ARG:HG3	1:A:277:ARG:HH11	1.60	0.67
1:B:106:PRO:HG2	1:B:109:GLY:HA3	1.77	0.66
1:C:228:ASN:ND2	1:C:230:ASP:H	1.90	0.66
1:C:236:LEU:CB	1:C:247:ILE:HG23	2.23	0.65
1:C:208:PRO:CG	1:C:291:SER:HA	2.27	0.65
1:C:27:ARG:HH11	2:C:1011:MPD:H31	1.62	0.63
1:C:10:GLN:HG2	3:C:1126:HOH:O	1.97	0.63
1:A:169:GLY:HA2	2:A:1003:MPD:H4	1.81	0.63
1:C:92:LYS:HA	1:C:264:VAL:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ILE:HG12	1:A:147:ILE:CD1	2.30	0.62
1:C:27:ARG:HD3	2:C:1011:MPD:H31	1.81	0.62
1:C:57:PHE:O	1:C:101:PRO:HG3	2.00	0.61
1:B:317:TYR:HA	3:B:1107:HOH:O	2.00	0.61
1:C:2:GLY:HA3	1:C:159:ARG:O	2.00	0.61
1:B:219:VAL:HG22	1:B:270:ALA:HB1	1.82	0.61
1:C:247:ILE:HD12	1:C:279:TYR:CE2	2.36	0.60
1:D:242:VAL:O	1:D:244:THR:HG22	2.02	0.59
1:B:37:GLN:HB3	1:B:39:ILE:HD11	1.85	0.59
1:A:42:ILE:HG12	1:A:147:ILE:HD13	1.83	0.59
1:A:116:MSE:HE3	3:A:1049:HOH:O	2.03	0.59
1:A:220:ILE:O	1:A:304:ASP:HB3	2.03	0.58
1:C:219:VAL:HG22	1:C:270:ALA:HB1	1.84	0.58
1:D:32:ARG:HD3	1:D:158:GLU:OE1	2.02	0.58
1:A:249:VAL:HG12	1:A:250:SER:O	2.02	0.58
1:C:212:TYR:HB2	1:C:284:LEU:HB3	1.84	0.58
1:A:9:LEU:HD11	1:A:155:ILE:HD12	1.85	0.58
1:C:213:LYS:HE2	1:C:214:ARG:NH2	2.19	0.58
1:D:236:LEU:CB	1:D:247:ILE:HG23	2.32	0.58
1:D:83:LEU:O	1:D:87:MSE:HG2	2.04	0.57
1:C:291:SER:HB2	2:C:1008:MPD:HM3	1.84	0.57
1:C:105:VAL:HG13	1:C:111:VAL:HG23	1.87	0.57
1:B:57:PHE:O	1:B:101:PRO:HG3	2.04	0.57
1:B:44:ASN:HD22	1:B:46:GLY:H	1.52	0.57
1:D:218:TYR:HA	1:D:270:ALA:O	2.05	0.56
1:D:213:LYS:HE3	1:D:214:ARG:HH12	1.69	0.56
1:C:254:LEU:HD23	1:C:254:LEU:O	2.06	0.56
1:B:261:GLU:HG3	1:B:278:LYS:CE	2.35	0.56
1:C:8:THR:HA	1:C:154:THR:HA	1.88	0.55
1:D:214:ARG:HG3	1:D:311:VAL:HB	1.89	0.55
1:C:98:TYR:O	1:C:113:LEU:HD12	2.06	0.55
1:B:68:SER:HB2	1:B:73:LYS:O	2.07	0.54
1:B:202:HIS:HA	1:B:297:ASP:OD1	2.08	0.54
1:A:121:LEU:HA	1:A:184:PRO:HG3	1.88	0.54
1:C:251:TRP:O	1:C:255:GLN:HG3	2.08	0.54
1:B:92:LYS:HG3	1:B:262:TYR:O	2.09	0.53
1:B:261:GLU:HG3	1:B:278:LYS:HZ1	1.73	0.53
1:A:57:PHE:O	1:A:101:PRO:HG3	2.07	0.52
1:B:274:ILE:N	1:B:274:ILE:HD12	2.24	0.52
1:D:43:SER:O	1:D:145:VAL:HG22	2.08	0.52
1:B:67:LEU:HD13	1:B:75:LEU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ARG:HG3	1:C:278:LYS:HD2	1.92	0.52
1:B:212:TYR:CE2	1:B:286:LEU:HD12	2.45	0.52
1:C:218:TYR:OH	2:C:1013:MPD:H13	2.09	0.52
1:C:91:THR:O	1:C:94:GLN:HG2	2.09	0.52
1:A:35:ARG:HD3	1:A:116:MSE:HE2	1.92	0.51
1:B:286:LEU:HD11	1:B:294:ILE:HD11	1.90	0.51
1:B:206:LEU:HD22	1:B:294:ILE:HD11	1.91	0.51
1:B:173:ALA:N	3:B:1152:HOH:O	2.16	0.51
1:D:35:ARG:HD3	1:D:116:MSE:HE2	1.91	0.51
1:B:207:GLN:HB2	3:B:1116:HOH:O	2.10	0.51
1:A:164:GLU:O	1:A:168:GLU:HG3	2.11	0.51
1:A:241:GLY:O	1:A:243:PRO:HD3	2.11	0.51
1:C:202:HIS:HA	1:C:297:ASP:OD2	2.10	0.51
1:A:181:THR:O	1:A:316:PRO:HD2	2.10	0.51
1:C:261:GLU:HG3	1:C:278:LYS:HZ1	1.75	0.51
1:B:238:ILE:HD11	1:B:246:LYS:HE2	1.92	0.50
1:C:218:TYR:HA	1:C:270:ALA:O	2.11	0.50
1:D:54:SER:HA	1:D:101:PRO:HB2	1.93	0.50
1:B:44:ASN:HD22	1:B:44:ASN:C	2.15	0.50
1:B:233:GLU:OE2	1:B:248:LYS:HE2	2.11	0.50
1:C:239:VAL:HG12	1:C:239:VAL:O	2.12	0.50
1:A:195:PRO:HG2	1:A:201:ILE:CD1	2.41	0.50
1:B:92:LYS:HD2	1:B:92:LYS:N	2.26	0.50
1:D:249:VAL:CG2	1:D:253:ALA:HB3	2.42	0.50
1:B:206:LEU:HD22	1:B:294:ILE:CD1	2.42	0.50
1:C:67:LEU:HB3	1:C:76:TYR:HB2	1.94	0.50
1:D:309:LEU:C	1:D:309:LEU:HD23	2.32	0.50
1:A:305:ASN:HD21	2:A:1005:MPD:C5	2.18	0.50
1:A:277:ARG:HG3	1:A:277:ARG:NH1	2.27	0.50
1:A:83:LEU:O	1:A:87:MSE:HG2	2.13	0.49
1:D:81:THR:HB	2:D:1015:MPD:H52	1.94	0.49
1:D:42:ILE:HG22	1:D:145:VAL:HG21	1.95	0.49
1:B:179:LEU:HD22	1:B:321:LEU:CD1	2.43	0.49
1:B:3:GLU:O	1:B:158:GLU:HA	2.13	0.49
1:A:128:MSE:HE2	1:A:176:GLU:O	2.13	0.48
1:D:15:TRP:CH2	1:D:147:ILE:HD12	2.48	0.48
1:C:31:ILE:CG2	1:C:121:LEU:HD22	2.43	0.48
1:C:56:PRO:HG2	1:C:60:ASN:ND2	2.28	0.48
1:B:235:GLU:HG2	1:B:297:ASP:HB2	1.95	0.48
1:C:61:LEU:HD12	1:C:61:LEU:HA	1.72	0.48
1:A:246:LYS:HE2	1:A:280:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLU:HG3	1:B:249:VAL:O	2.14	0.48
1:C:307:TYR:CZ	2:C:1013:MPD:H11	2.48	0.47
1:B:213:LYS:HG3	1:B:277:ARG:NH1	2.28	0.47
1:A:249:VAL:CG1	1:A:253:ALA:HB3	2.44	0.47
1:C:309:LEU:C	1:C:309:LEU:HD23	2.35	0.47
1:C:56:PRO:HG2	1:C:60:ASN:HD22	1.79	0.47
1:A:249:VAL:HG12	1:A:250:SER:N	2.29	0.47
1:D:2:GLY:HA3	1:D:159:ARG:O	2.14	0.47
1:D:274:ILE:N	1:D:274:ILE:HD12	2.30	0.47
1:D:219:VAL:HG21	1:D:231:PRO:HD3	1.96	0.46
1:B:249:VAL:HG22	1:B:250:SER:O	2.15	0.46
1:C:213:LYS:HE2	1:C:214:ARG:HH21	1.80	0.46
1:C:275:ASP:HB2	1:C:278:LYS:HD3	1.98	0.46
1:C:307:TYR:CE2	2:C:1013:MPD:H11	2.51	0.46
1:D:174:ASP:CG	1:D:176:GLU:HG3	2.35	0.46
1:D:195:PRO:HG2	1:D:201:ILE:CD1	2.46	0.46
1:A:277:ARG:HA	1:A:282:GLY:O	2.15	0.46
1:C:44:ASN:ND2	1:C:46:GLY:H	2.14	0.46
1:D:116:MSE:HE3	3:D:1070:HOH:O	2.16	0.46
1:C:154:THR:HG23	3:C:1113:HOH:O	2.14	0.46
1:D:315:LEU:HD12	1:D:318:TYR:HD1	1.81	0.46
1:A:218:TYR:HA	1:A:270:ALA:O	2.16	0.45
1:D:218:TYR:OH	2:D:1015:MPD:H51	2.15	0.45
1:C:123:ARG:HD2	1:C:158:GLU:OE2	2.16	0.45
1:C:76:TYR:CZ	1:C:186:VAL:HG21	2.51	0.45
1:C:233:GLU:HG3	1:C:234:TYR:N	2.31	0.45
1:A:24:LYS:CE	1:A:131:ASN:HA	2.45	0.45
1:D:63:GLN:HG2	1:D:64:THR:HG23	1.99	0.45
1:B:121:LEU:HA	1:B:184:PRO:HG3	1.98	0.45
1:C:68:SER:HB2	1:C:73:LYS:O	2.17	0.45
1:C:92:LYS:HA	1:C:264:VAL:CG2	2.47	0.45
1:B:69:TYR:HD2	1:B:70:GLU:HG3	1.81	0.44
1:C:8:THR:HG23	1:C:154:THR:HG22	1.98	0.44
1:C:212:TYR:CE2	1:C:286:LEU:HD12	2.52	0.44
1:C:8:THR:CB	1:C:154:THR:HG22	2.47	0.44
1:C:106:PRO:HG2	1:C:109:GLY:HA3	1.99	0.44
1:B:67:LEU:HD13	1:B:75:LEU:HD12	1.99	0.44
1:C:188:GLU:HA	1:C:309:LEU:HA	1.99	0.44
1:C:213:LYS:HD2	2:C:1012:MPD:H12	1.98	0.44
1:D:249:VAL:HG22	1:D:250:SER:O	2.18	0.44
1:B:44:ASN:ND2	1:B:44:ASN:C	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:VAL:HG22	3:B:1105:HOH:O	2.17	0.44
1:B:96:PRO:HG2	1:B:116:MSE:HB3	2.00	0.44
1:B:208:PRO:HG2	1:B:291:SER:HA	1.99	0.44
1:D:220:ILE:O	1:D:304:ASP:HB3	2.18	0.44
1:B:163:GLN:NE2	1:B:167:SER:HB3	2.33	0.43
1:A:230:ASP:N	1:A:231:PRO:HD2	2.33	0.43
1:B:218:TYR:HA	1:B:270:ALA:O	2.19	0.43
1:B:235:GLU:OE2	1:B:248:LYS:HD3	2.19	0.43
1:B:28:ASN:O	1:B:29:ASN:CG	2.57	0.43
1:C:254:LEU:CD2	1:C:272:ALA:HB1	2.43	0.43
1:D:322:ALA:C	1:D:324:LEU:H	2.20	0.43
1:B:286:LEU:HD11	1:B:294:ILE:CD1	2.49	0.42
1:A:213:LYS:HE2	1:A:214:ARG:NH2	2.34	0.42
1:B:8:THR:HA	1:B:154:THR:HA	2.01	0.42
1:B:66:ASN:HB3	1:B:135:SER:HB2	2.02	0.42
1:C:274:ILE:HD12	1:C:274:ILE:N	2.34	0.42
2:A:1003:MPD:H31	3:A:1056:HOH:O	2.18	0.42
1:C:92:LYS:HD3	1:C:263:GLN:NE2	2.34	0.42
1:D:76:TYR:CD1	1:D:186:VAL:HB	2.54	0.42
1:A:35:ARG:HB3	1:A:154:THR:HB	2.01	0.42
1:A:63:GLN:HG2	1:A:64:THR:HG23	2.01	0.42
1:C:39:ILE:C	1:C:39:ILE:HD12	2.41	0.42
1:A:98:TYR:CZ	1:D:94:GLN:HG2	2.54	0.41
1:B:230:ASP:OD1	1:B:304:ASP:OD1	2.37	0.41
1:C:53:PRO:HG2	1:C:57:PHE:CG	2.55	0.41
1:C:63:GLN:HG2	1:C:64:THR:HG23	2.02	0.41
1:A:249:VAL:CG1	1:A:250:SER:N	2.83	0.41
1:B:39:ILE:CD1	1:B:114:ASN:ND2	2.83	0.41
1:C:94:GLN:O	1:C:95:ASN:C	2.59	0.41
1:A:214:ARG:HG2	1:A:311:VAL:HB	2.03	0.41
1:B:179:LEU:HD22	1:B:321:LEU:HD13	2.02	0.41
2:D:1015:MPD:H32	3:D:1135:HOH:O	2.20	0.41
1:C:251:TRP:CH2	1:C:272:ALA:HB3	2.55	0.41
1:C:303:GLN:HE21	1:C:303:GLN:HB2	1.69	0.41
1:D:246:LYS:HD3	1:D:246:LYS:HA	1.88	0.41
1:C:202:HIS:HD2	1:C:295:GLU:OE1	2.03	0.41
1:C:254:LEU:HD23	1:C:254:LEU:C	2.40	0.41
1:B:76:TYR:CD1	1:B:186:VAL:HB	2.55	0.41
1:C:95:ASN:OD1	1:C:116:MSE:HE2	2.20	0.41
1:D:246:LYS:C	1:D:247:ILE:HG22	2.41	0.41
1:A:293:SER:HB2	3:A:1164:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.93	0.41
1:B:96:PRO:HG2	1:B:116:MSE:CB	2.51	0.41
1:D:121:LEU:HA	1:D:184:PRO:HG3	2.03	0.41
1:A:218:TYR:OH	2:A:1001:MPD:H52	2.20	0.41
1:C:5:TYR:CE1	1:C:157:TYR:HB2	2.56	0.41
1:C:58:PRO:O	1:C:61:LEU:HB2	2.21	0.41
1:D:174:ASP:OD1	1:D:176:GLU:HG3	2.21	0.41
1:D:186:VAL:O	1:D:187:ILE:HD13	2.21	0.41
1:D:208:PRO:CG	1:D:291:SER:HA	2.51	0.41
1:A:24:LYS:HE2	3:A:1024:HOH:O	2.20	0.41
1:B:213:LYS:HG3	1:B:277:ARG:HH12	1.86	0.41
1:B:309:LEU:C	1:B:309:LEU:HD23	2.41	0.41
1:A:24:LYS:HZ3	1:A:24:LYS:HG2	1.77	0.40
1:C:172:GLY:HA3	1:C:317:TYR:CE2	2.57	0.40
1:C:230:ASP:N	1:C:231:PRO:CD	2.84	0.40
1:D:43:SER:O	1:D:145:VAL:CG2	2.69	0.40
1:C:246:LYS:C	1:C:247:ILE:HG22	2.42	0.40
2:C:1008:MPD:H31	3:C:1144:HOH:O	2.21	0.40
1:A:309:LEU:C	1:A:309:LEU:HD23	2.41	0.40
1:B:25:ILE:HG23	1:B:155:ILE:HD13	2.03	0.40
1:B:212:TYR:HE2	1:B:286:LEU:HD12	1.84	0.40
1:B:320:GLN:CD	3:B:1152:HOH:O	2.60	0.40
1:B:320:GLN:OE1	3:B:1152:HOH:O	2.22	0.40
1:C:119:PHE:CD1	1:C:119:PHE:N	2.89	0.40
1:C:177:MSE:HE1	1:C:183:LEU:HD11	2.03	0.40
1:A:184:PRO:HB3	2:A:1002:MPD:H11	2.02	0.40
1:A:319:ASP:O	1:A:322:ALA:HB3	2.21	0.40
1:B:32:ARG:HD2	1:B:158:GLU:OE2	2.22	0.40
1:B:321:LEU:HD12	1:B:321:LEU:HA	1.91	0.40
1:D:50:VAL:HG13	1:D:105:VAL:HB	2.02	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	321/350 (92%)	305 (95%)	16 (5%)	0	100	100
1	B	321/350 (92%)	308 (96%)	11 (3%)	2 (1%)	22	13
1	C	321/350 (92%)	303 (94%)	16 (5%)	2 (1%)	22	13
1	D	321/350 (92%)	306 (95%)	15 (5%)	0	100	100
All	All	1284/1400 (92%)	1222 (95%)	58 (4%)	4 (0%)	37	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	291	SER
1	B	131	ASN
1	B	245	ASP
1	C	131	ASN

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	271/291 (93%)	270 (100%)	1 (0%)	89	91
1	B	272/291 (94%)	262 (96%)	10 (4%)	29	23
1	C	271/291 (93%)	262 (97%)	9 (3%)	33	27
1	D	271/291 (93%)	262 (97%)	9 (3%)	33	27
All	All	1085/1164 (93%)	1056 (97%)	29 (3%)	40	35

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

Mol	Chain	Res	Type
1	A	171	LEU
1	B	10	GLN
1	B	44	ASN
1	B	60	ASN

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Mol	Chain	Res	Type
1	B	67	LEU
1	B	92	LYS
1	B	159	ARG
1	B	166	LEU
1	B	179	LEU
1	B	245	ASP
1	B	321	LEU
1	C	44	ASN
1	C	61	LEU
1	C	86	LEU
1	C	146	SER
1	C	233	GLU
1	C	247	ILE
1	C	264	VAL
1	C	268	SER
1	C	281	ASN
1	D	6	THR
1	D	86	LEU
1	D	90	THR
1	D	114	ASN
1	D	145	VAL
1	D	148	ASN
1	D	223	THR
1	D	244	THR
1	D	247	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	28	ASN
1	A	94	GLN
1	A	95	ASN
1	A	131	ASN
1	A	215	GLN
1	B	28	ASN
1	B	44	ASN
1	B	60	ASN
1	B	114	ASN
1	B	131	ASN
1	B	140	GLN
1	B	163	GLN

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Mol	Chain	Res	Type
1	B	193	ASN
1	B	215	GLN
1	B	227	ASN
1	B	263	GLN
1	C	29	ASN
1	C	37	GLN
1	C	44	ASN
1	C	207	GLN
1	C	215	GLN
1	C	228	ASN
1	C	263	GLN
1	C	281	ASN
1	C	303	GLN
1	D	10	GLN
1	D	11	GLN
1	D	28	ASN
1	D	29	ASN
1	D	66	ASN
1	D	114	ASN
1	D	131	ASN
1	D	215	GLN
1	D	227	ASN
1	D	228	ASN
1	D	281	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MPD	A	1001	-	7,7,7	0.45	0	9,10,10	0.80	0
2	MPD	A	1014	-	7,7,7	0.55	0	9,10,10	0.46	0
2	MPD	B	1010	-	7,7,7	0.46	0	9,10,10	0.65	0
2	MPD	A	1002	-	7,7,7	0.51	0	9,10,10	0.47	0
2	MPD	C	1013	-	7,7,7	0.56	0	9,10,10	0.61	0
2	MPD	A	1006	-	7,7,7	0.55	0	9,10,10	0.47	0
2	MPD	A	1009	-	7,7,7	0.39	0	9,10,10	0.63	0
2	MPD	D	1016	-	7,7,7	0.49	0	9,10,10	0.62	0
2	MPD	C	1008	-	7,7,7	0.59	0	9,10,10	0.60	0
2	MPD	A	1005	-	7,7,7	0.42	0	9,10,10	0.63	0
2	MPD	D	1017	-	7,7,7	0.41	0	9,10,10	0.49	0
2	MPD	A	1004	-	7,7,7	0.46	0	9,10,10	0.69	0
2	MPD	C	1007	-	7,7,7	0.45	0	9,10,10	0.46	0
2	MPD	A	1003	-	7,7,7	0.59	0	9,10,10	0.65	0
2	MPD	C	1012	-	7,7,7	0.51	0	9,10,10	0.48	0
2	MPD	D	1015	-	7,7,7	0.46	0	9,10,10	0.70	0
2	MPD	C	1011	-	7,7,7	0.45	0	9,10,10	0.56	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	MPD	A	1001	-	-	1/5/5/5	-
2	MPD	A	1014	-	-	3/5/5/5	-
2	MPD	B	1010	-	-	1/5/5/5	-
2	MPD	A	1002	-	-	0/5/5/5	-
2	MPD	C	1013	-	-	0/5/5/5	-
2	MPD	A	1006	-	-	3/5/5/5	-
2	MPD	A	1009	-	-	1/5/5/5	-
2	MPD	D	1016	-	-	1/5/5/5	-
2	MPD	C	1008	-	-	1/5/5/5	-
2	MPD	A	1005	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	D	1017	-	-	3/5/5/5	-
2	MPD	A	1004	-	-	1/5/5/5	-
2	MPD	C	1007	-	-	2/5/5/5	-
2	MPD	A	1003	-	-	1/5/5/5	-
2	MPD	C	1012	-	-	1/5/5/5	-
2	MPD	D	1015	-	-	1/5/5/5	-
2	MPD	C	1011	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1005	MPD	O2-C2-C3-C4
2	A	1009	MPD	O2-C2-C3-C4
2	B	1010	MPD	O2-C2-C3-C4
2	C	1011	MPD	O2-C2-C3-C4
2	D	1016	MPD	O2-C2-C3-C4
2	A	1006	MPD	C1-C2-C3-C4
2	A	1006	MPD	CM-C2-C3-C4
2	A	1014	MPD	CM-C2-C3-C4
2	A	1001	MPD	O2-C2-C3-C4
2	A	1003	MPD	O2-C2-C3-C4
2	A	1004	MPD	O2-C2-C3-C4
2	A	1006	MPD	O2-C2-C3-C4
2	A	1014	MPD	O2-C2-C3-C4
2	C	1008	MPD	O2-C2-C3-C4
2	C	1012	MPD	O2-C2-C3-C4
2	D	1015	MPD	O2-C2-C3-C4
2	D	1017	MPD	O2-C2-C3-C4
2	A	1014	MPD	C1-C2-C3-C4
2	C	1007	MPD	C1-C2-C3-C4
2	C	1007	MPD	CM-C2-C3-C4
2	D	1017	MPD	C1-C2-C3-C4
2	D	1017	MPD	CM-C2-C3-C4

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	MPD	1	0
2	A	1002	MPD	1	0
2	C	1013	MPD	3	0
2	C	1008	MPD	2	0
2	A	1005	MPD	2	0
2	A	1003	MPD	2	0
2	C	1012	MPD	1	0
2	D	1015	MPD	3	0
2	C	1011	MPD	2	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	319/350 (91%)	-0.15	6 (1%) 66 69	19, 28, 43, 62	0
1	B	319/350 (91%)	0.47	10 (3%) 51 53	23, 39, 53, 59	0
1	C	319/350 (91%)	0.57	15 (4%) 37 40	25, 41, 54, 59	0
1	D	319/350 (91%)	-0.05	8 (2%) 58 60	20, 30, 44, 60	0
All	All	1276/1400 (91%)	0.21	39 (3%) 51 53	19, 35, 52, 62	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	291	SER	4.9
1	B	324	LEU	4.7
1	C	323	ALA	4.6
1	A	324	LEU	4.0
1	D	322	ALA	3.8
1	C	148	ASN	3.7
1	A	323	ALA	3.6
1	D	324	LEU	3.4
1	C	324	LEU	3.3
1	D	247	ILE	3.1
1	B	160	VAL	3.1
1	B	111	VAL	3.0
1	D	323	ALA	2.8
1	D	180	ALA	2.5
1	B	149	ALA	2.5
1	C	214	ARG	2.5
1	C	277	ARG	2.5
1	A	24	LYS	2.4
1	B	159	ARG	2.4
1	B	281	ASN	2.3
1	A	320	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	321	LEU	2.3
1	C	321	LEU	2.3
1	B	323	ALA	2.3
1	C	49	ALA	2.3
1	C	149	ALA	2.3
1	B	241	GLY	2.3
1	A	322	ALA	2.2
1	C	322	ALA	2.2
1	D	277	ARG	2.2
1	C	109	GLY	2.2
1	B	294	ILE	2.1
1	C	47	THR	2.1
1	B	244	THR	2.1
1	C	270	ALA	2.1
1	C	46	GLY	2.1
1	A	242	VAL	2.0
1	D	242	VAL	2.0
1	C	282	GLY	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MPD	A	1005	8/8	0.64	0.24	57,59,60,61	0
2	MPD	A	1003	8/8	0.65	0.23	53,56,57,58	0
2	MPD	D	1015	8/8	0.68	0.34	35,45,51,55	0
2	MPD	C	1007	8/8	0.69	0.24	53,56,57,57	0
2	MPD	A	1004	8/8	0.69	0.25	45,50,53,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MPD	C	1008	8/8	0.70	0.25	55,57,60,61	0
2	MPD	B	1010	8/8	0.71	0.21	54,56,56,56	0
2	MPD	A	1001	8/8	0.72	0.22	32,33,38,41	0
2	MPD	A	1009	8/8	0.73	0.20	51,54,55,56	0
2	MPD	C	1011	8/8	0.76	0.21	54,55,56,58	0
2	MPD	D	1016	8/8	0.77	0.19	55,57,58,61	0
2	MPD	D	1017	8/8	0.82	0.17	51,53,54,56	0
2	MPD	A	1006	8/8	0.84	0.17	51,52,53,53	0
2	MPD	A	1002	8/8	0.86	0.12	49,50,52,53	0
2	MPD	C	1013	8/8	0.87	0.15	38,39,41,43	0
2	MPD	A	1014	8/8	0.87	0.18	55,55,56,57	0
2	MPD	C	1012	8/8	0.89	0.14	51,53,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.