



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:27 AM UTC

PDB ID : 2BBD / pdb_00002bbd
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

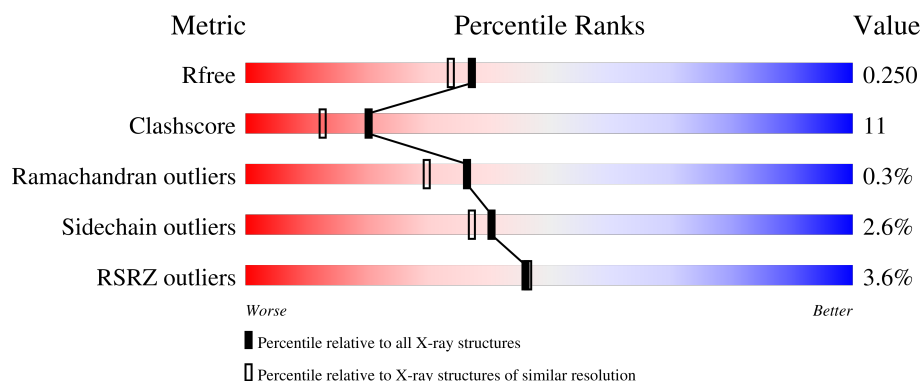
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 $\leq 5\%$. 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	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 8%</div> </div> </div>
1	B	350	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>• 8%</div> </div> </div>
1	C	350	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>24%</div> <div>• 8%</div> </div> </div>
1	D	350	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>• 8%</div> </div> </div>

2 Entry composition

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:

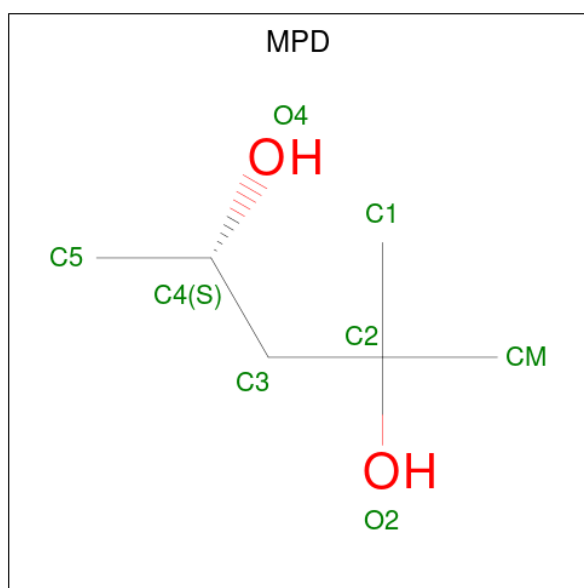
Chain	Residue	Modelled	Actual	Comment	Reference
A	87	MSE	MET	modified residue	UNP Q6Q0J0
A	116	MSE	MET	modified residue	UNP Q6Q0J0
A	128	MSE	MET	modified residue	UNP Q6Q0J0
A	177	MSE	MET	modified residue	UNP Q6Q0J0
A	346	HIS	-	expression tag	UNP Q6Q0J0
A	347	HIS	-	expression tag	UNP Q6Q0J0
A	348	HIS	-	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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

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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	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

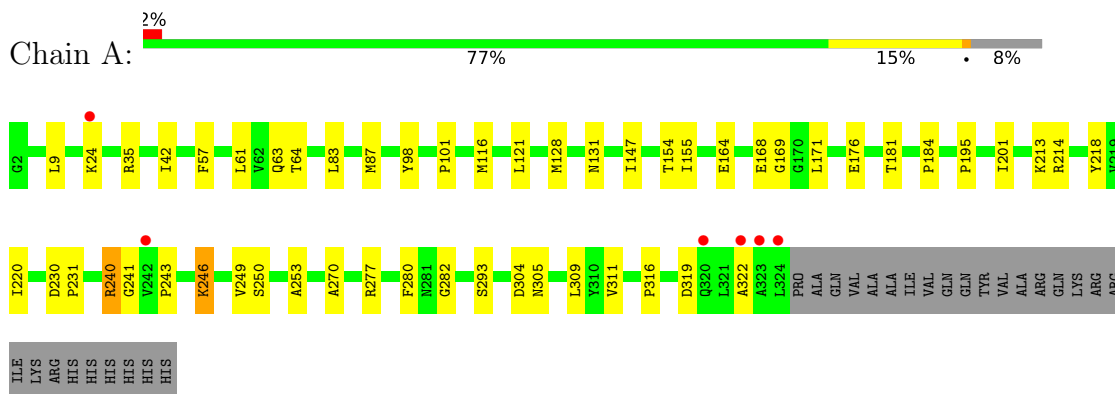
- Molecule 3 is water.

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
3	D	239	Total O 239 239	0	0

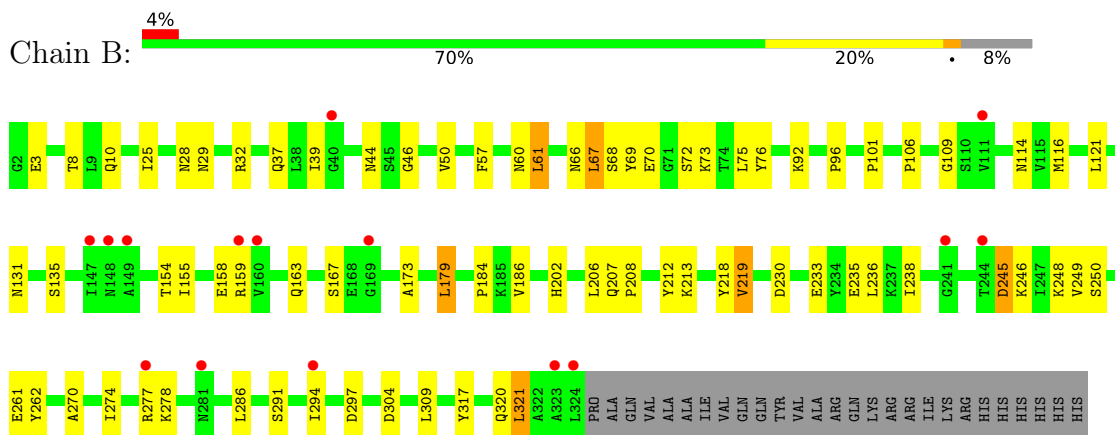
3 Residue-property plots [i](#)

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.

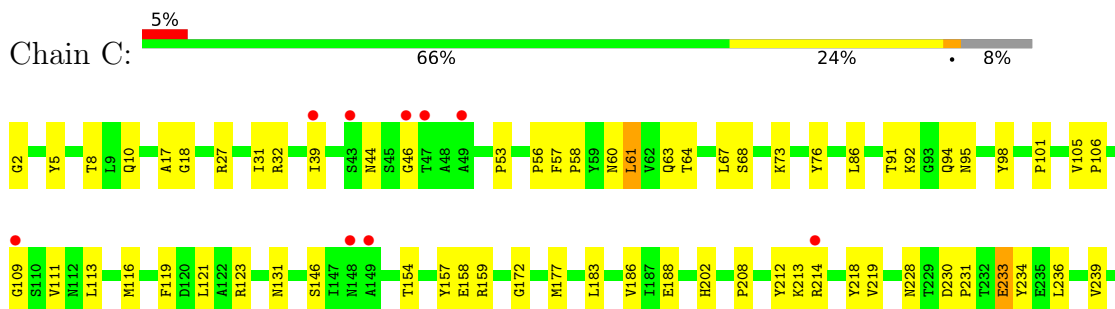
• Molecule 1: coat protein

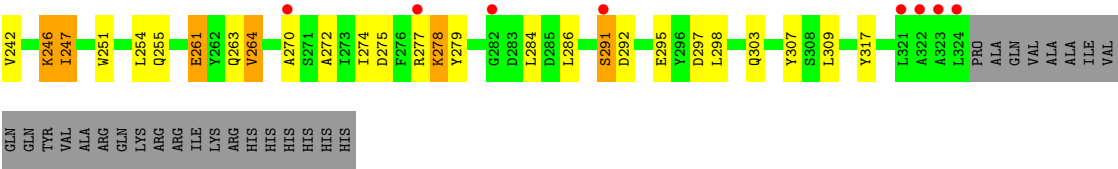


• Molecule 1: coat protein

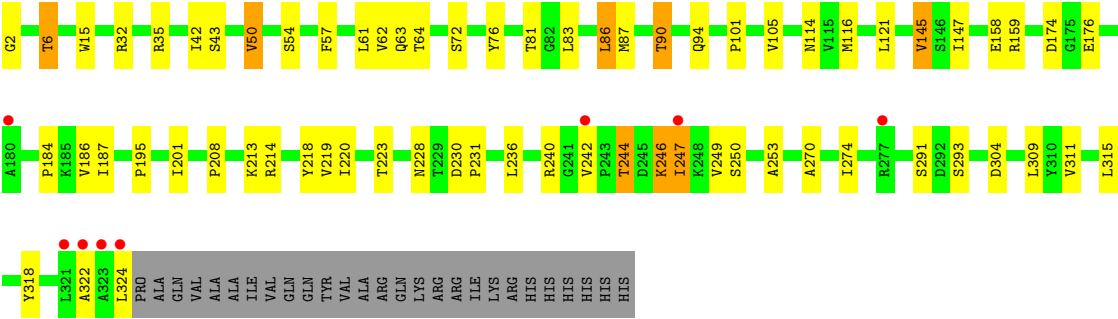


• Molecule 1: coat protein





● Molecule 1: coat protein



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.246 0.212 , 0.250	Depositor DCC
R_{free} test set	8014 reflections (7.03%)	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	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h-2*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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.41	0/2545	0.93	2/3480 (0.1%)
1	B	0.37	0/2548	0.90	3/3484 (0.1%)
1	C	0.37	0/2545	0.90	1/3480 (0.0%)
1	D	0.41	0/2545	0.92	5/3480 (0.1%)
All	All	0.39	0/10183	0.91	11/13924 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	246	LYS	N-CA-C	-6.22	106.01	113.97
1	A	246	LYS	N-CA-C	-6.15	106.09	113.97
1	B	61	LEU	N-CA-C	-6.14	105.65	113.01
1	A	61	LEU	N-CA-C	-5.83	106.13	113.18
1	D	61	LEU	N-CA-C	-5.66	106.22	113.01
1	D	72	SER	N-CA-C	5.58	120.98	113.72
1	D	62	VAL	N-CA-C	-5.50	100.41	108.11
1	C	246	LYS	N-CA-C	-5.45	106.63	113.28
1	B	236	LEU	N-CA-C	-5.19	100.78	109.24
1	D	57	PHE	N-CA-C	-5.11	103.03	110.08
1	B	72	SER	N-CA-C	5.04	119.42	113.28

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	42	0
1	B	2491	0	2466	59	0
1	C	2488	0	2457	78	0
1	D	2488	0	2457	46	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
3	B	143	0	0	5	0
3	C	143	0	0	5	0
3	D	239	0	0	2	0
All	All	10870	0	10075	227	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 (227) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ASN:HD22	1:B:44:ASN:C	2.15	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:D:309:LEU:C	1:D:309:LEU:HD23	2.32	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:A:57:PHE:O	1:A:101:PRO:HG3	2.07	0.52
1:C:261:GLU:HG3	1:C:278:LYS:HZ1	1.73	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
1:C:277:ARG:HG3	1:C:278:LYS:HD2	1.92	0.52
1:C:309:LEU:C	1:C:309:LEU:HD23	2.35	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:D:174:ASP:CG	1:D:176:GLU:HG3	2.35	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: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: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:A:305:ASN:HD21	2:A:1005:MPD:C5	2.18	0.50
1:B:44:ASN:ND2	1:B:44:ASN:C	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:233:GLU:HG3	1:B:249:VAL:O	2.14	0.48
1:D:322:ALA:C	1:D:324:LEU:H	2.20	0.48
1:C:307:TYR:CZ	2:C:1013:MPD:H11	2.48	0.47
1:B:28:ASN:O	1:B:29:ASN:CG	2.57	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: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:B:261:GLU:HG3	1:B:278:LYS:HZ3	1.79	0.46
1:C:39:ILE:C	1:C:39:ILE:HD12	2.41	0.46
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:254:LEU:HD23	1:C:254:LEU:C	2.40	0.46
1:C:94:GLN:O	1:C:95:ASN:C	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:LEU:C	1:B:309:LEU:HD23	2.41	0.45
1:B:320:GLN:CD	3:B:1152:HOH:O	2.60	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:C:246:LYS:C	1:C:247:ILE:HG22	2.42	0.45
1:A:24:LYS:CE	1:A:131:ASN:HA	2.45	0.45
1:A:309:LEU:C	1:A:309:LEU:HD23	2.41	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:B:261:GLU:HG3	1:B:278:LYS:HZ1	1.81	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:D:246:LYS:C	1:D:247:ILE:HG22	2.41	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: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:C:254:LEU:CD2	1:C:272:ALA:HB1	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:293:SER:HB2	3:A:1164:HOH:O	2.20	0.41
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:C:17:ALA:O	1:C:18:GLY:C	2.64	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:114:ASN:C	1:D:114:ASN:HD22	2.29	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:D:114:ASN:C	1:D:114:ASN:ND2	2.79	0.41
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:C:291:SER:C	3:C:1156:HOH:O	2.62	0.40
1:D:43:SER:O	1:D:145:VAL:CG2	2.69	0.40
2:C:1008:MPD:H31	3:C:1144:HOH:O	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	21	13
1	C	321/350 (92%)	303 (94%)	16 (5%)	2 (1%)	21	13
1	D	321/350 (92%)	306 (95%)	15 (5%)	0	100	100
All	All	1284/1400 (92%)	1222 (95%)	58 (4%)	4 (0%)	36	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%)	269 (99%)	2 (1%)	76	80
1	B	272/291 (94%)	264 (97%)	8 (3%)	37	33
1	C	271/291 (93%)	261 (96%)	10 (4%)	30	25
1	D	271/291 (93%)	263 (97%)	8 (3%)	36	32
All	All	1085/1164 (93%)	1057 (97%)	28 (3%)	40	37

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

Mol	Chain	Res	Type
1	A	171	LEU
1	A	240	ARG
1	B	10	GLN
1	B	60	ASN
1	B	67	LEU
1	B	159	ARG
1	B	179	LEU
1	B	219	VAL
1	B	245	ASP
1	B	321	LEU
1	C	61	LEU
1	C	86	LEU
1	C	146	SER
1	C	233	GLU
1	C	242	VAL
1	C	247	ILE
1	C	261	GLU
1	C	264	VAL
1	C	278	LYS
1	C	298	LEU
1	D	6	THR
1	D	50	VAL
1	D	86	LEU
1	D	90	THR
1	D	145	VAL
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 (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	28	ASN
1	A	94	GLN
1	A	112	ASN
1	A	131	ASN
1	A	207	GLN
1	A	215	GLN
1	A	227	ASN
1	A	263	GLN
1	A	281	ASN
1	A	301	GLN
1	B	11	GLN
1	B	28	ASN
1	B	44	ASN
1	B	60	ASN
1	B	114	ASN
1	B	140	GLN
1	B	148	ASN
1	B	163	GLN
1	B	215	GLN
1	B	263	GLN
1	B	301	GLN
1	C	20	ASN
1	C	29	ASN
1	C	44	ASN
1	C	60	ASN
1	C	207	GLN
1	C	210	GLN
1	C	215	GLN
1	C	228	ASN
1	C	263	GLN
1	C	281	ASN
1	C	301	GLN
1	C	302	ASN
1	C	303	GLN
1	D	10	GLN
1	D	11	GLN
1	D	29	ASN
1	D	114	ASN
1	D	131	ASN
1	D	148	ASN
1	D	215	GLN
1	D	227	ASN

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Mol	Chain	Res	Type
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	1005	-	7,7,7	0.42	0	9,10,10	0.63	0
2	MPD	A	1006	-	7,7,7	0.55	0	9,10,10	0.47	0
2	MPD	C	1008	-	7,7,7	0.59	0	9,10,10	0.60	0
2	MPD	D	1016	-	7,7,7	0.49	0	9,10,10	0.62	0
2	MPD	A	1002	-	7,7,7	0.51	0	9,10,10	0.47	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	A	1004	-	7,7,7	0.46	0	9,10,10	0.69	0
2	MPD	C	1012	-	7,7,7	0.51	0	9,10,10	0.48	0
2	MPD	A	1014	-	7,7,7	0.55	0	9,10,10	0.46	0
2	MPD	C	1011	-	7,7,7	0.45	0	9,10,10	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MPD	D	1017	-	7,7,7	0.41	0	9,10,10	0.49	0
2	MPD	B	1010	-	7,7,7	0.46	0	9,10,10	0.65	0
2	MPD	D	1015	-	7,7,7	0.46	0	9,10,10	0.70	0
2	MPD	A	1009	-	7,7,7	0.39	0	9,10,10	0.63	0
2	MPD	C	1013	-	7,7,7	0.56	0	9,10,10	0.61	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	1005	-	-	1/5/5/5	-
2	MPD	A	1006	-	-	3/5/5/5	-
2	MPD	C	1008	-	-	1/5/5/5	-
2	MPD	D	1016	-	-	1/5/5/5	-
2	MPD	A	1002	-	-	0/5/5/5	-
2	MPD	C	1007	-	-	2/5/5/5	-
2	MPD	A	1003	-	-	1/5/5/5	-
2	MPD	A	1004	-	-	1/5/5/5	-
2	MPD	C	1012	-	-	1/5/5/5	-
2	MPD	A	1014	-	-	3/5/5/5	-
2	MPD	C	1011	-	-	1/5/5/5	-
2	MPD	D	1017	-	-	3/5/5/5	-
2	MPD	B	1010	-	-	1/5/5/5	-
2	MPD	D	1015	-	-	1/5/5/5	-
2	MPD	A	1009	-	-	1/5/5/5	-
2	MPD	C	1013	-	-	0/5/5/5	-

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

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Mol	Chain	Res	Type	Atoms
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	1005	MPD	2	0
2	C	1008	MPD	2	0
2	A	1002	MPD	1	0
2	A	1003	MPD	2	0
2	C	1012	MPD	1	0
2	C	1011	MPD	2	0
2	D	1015	MPD	3	0
2	C	1013	MPD	3	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, 95th 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%)	-0.04	6 (1%) 66 68	19, 28, 43, 62	0
1	B	319/350 (91%)	0.58	15 (4%) 36 36	23, 39, 53, 59	0
1	C	319/350 (91%)	0.68	17 (5%) 32 32	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%)	0.32	46 (3%) 46 46	19, 35, 52, 62	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	291	SER	5.0
1	B	324	LEU	4.9
1	C	323	ALA	4.8
1	A	324	LEU	4.2
1	D	322	ALA	4.0
1	C	148	ASN	3.8
1	A	323	ALA	3.8
1	D	324	LEU	3.6
1	C	324	LEU	3.5
1	D	247	ILE	3.3
1	B	160	VAL	3.2
1	B	111	VAL	3.2
1	D	323	ALA	3.0
1	D	180	ALA	2.7
1	B	149	ALA	2.7
1	C	214	ARG	2.6
1	C	277	ARG	2.5
1	D	321	LEU	2.5
1	B	281	ASN	2.5
1	B	323	ALA	2.4
1	C	49	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	149	ALA	2.4
1	A	24	LYS	2.4
1	C	321	LEU	2.4
1	B	159	ARG	2.4
1	B	241	GLY	2.4
1	A	320	GLN	2.4
1	A	322	ALA	2.4
1	C	322	ALA	2.3
1	C	109	GLY	2.3
1	D	277	ARG	2.3
1	B	294	ILE	2.2
1	C	47	THR	2.2
1	C	46	GLY	2.2
1	C	270	ALA	2.2
1	B	244	THR	2.2
1	A	242	VAL	2.2
1	D	242	VAL	2.2
1	C	282	GLY	2.2
1	B	147	ILE	2.1
1	B	148	ASN	2.1
1	B	169	GLY	2.1
1	B	40	GLY	2.0
1	C	39	ILE	2.0
1	C	43	SER	2.0
1	B	277	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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(\AA^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
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

There are no such residues in this entry.