



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 10:53 AM BST

PDB ID : 6BHK
Title : Phosphotriesterase variant R18deltaL7
Authors : Miton, C.M.; Campbell, E.C.; Jackson, C.J.; Tokuriki, N.
Deposited on : 2017-10-30
Resolution : 1.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

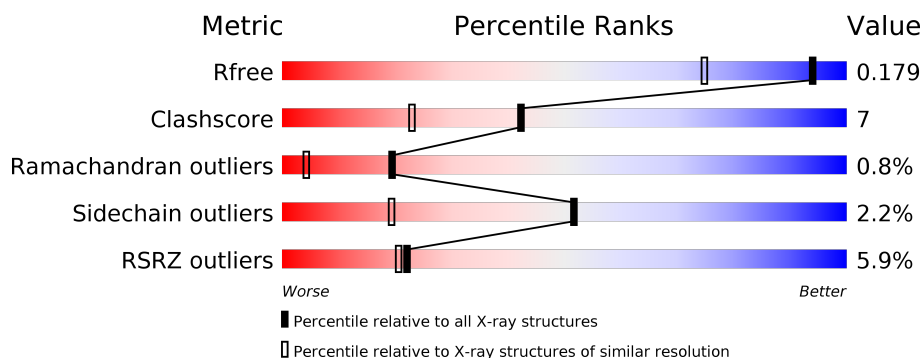
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 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	324	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	B	324	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
1	E	324	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	G	324	<div> <div>6%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>.</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22639 atoms, of which 10973 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 Phosphotriesterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	318	Total	C	H	N	O	S	0	39	0
			5346	1664	2703	481	490	8			
1	G	316	Total	C	H	N	O	S	0	34	0
			5254	1636	2660	476	474	8			
1	B	320	Total	C	H	N	O	S	0	26	0
			5242	1637	2652	468	476	9			
1	E	319	Total	C	H	N	O	S	0	49	0
			5430	1689	2748	491	494	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP A0A060GYS7
A	?	-	ALA	deletion	UNP A0A060GYS7
A	?	-	SER	deletion	UNP A0A060GYS7
A	?	-	ALA	deletion	UNP A0A060GYS7
A	?	-	THR	deletion	UNP A0A060GYS7
A	?	-	ALA	deletion	UNP A0A060GYS7
A	?	-	PHE	deletion	UNP A0A060GYS7
A	?	-	MET	deletion	UNP A0A060GYS7
A	?	-	GLY	deletion	UNP A0A060GYS7
G	?	-	ASN	deletion	UNP A0A060GYS7
G	?	-	ALA	deletion	UNP A0A060GYS7
G	?	-	SER	deletion	UNP A0A060GYS7
G	?	-	ALA	deletion	UNP A0A060GYS7
G	?	-	THR	deletion	UNP A0A060GYS7
G	?	-	ALA	deletion	UNP A0A060GYS7
G	?	-	PHE	deletion	UNP A0A060GYS7
G	?	-	MET	deletion	UNP A0A060GYS7
G	?	-	GLY	deletion	UNP A0A060GYS7
B	?	-	ASN	deletion	UNP A0A060GYS7
B	?	-	ALA	deletion	UNP A0A060GYS7
B	?	-	SER	deletion	UNP A0A060GYS7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ALA	deletion	UNP A0A060GYS7
B	?	-	THR	deletion	UNP A0A060GYS7
B	?	-	ALA	deletion	UNP A0A060GYS7
B	?	-	PHE	deletion	UNP A0A060GYS7
B	?	-	MET	deletion	UNP A0A060GYS7
B	?	-	GLY	deletion	UNP A0A060GYS7
E	?	-	ASN	deletion	UNP A0A060GYS7
E	?	-	ALA	deletion	UNP A0A060GYS7
E	?	-	SER	deletion	UNP A0A060GYS7
E	?	-	ALA	deletion	UNP A0A060GYS7
E	?	-	THR	deletion	UNP A0A060GYS7
E	?	-	ALA	deletion	UNP A0A060GYS7
E	?	-	PHE	deletion	UNP A0A060GYS7
E	?	-	MET	deletion	UNP A0A060GYS7
E	?	-	GLY	deletion	UNP A0A060GYS7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			22	6	14	2		
3	A	1	Total	C	H	O	0	0
			22	6	14	2		
3	A	1	Total	C	H	O	0	0
			22	6	14	2		
3	G	1	Total	C	H	O	0	1
			44	12	28	4		
3	G	1	Total	C	H	O	0	0
			22	6	14	2		
3	G	1	Total	C	H	O	0	0
			22	6	14	2		
3	G	1	Total	C	H	O	0	0
			22	6	14	2		
3	B	1	Total	C	H	O	0	0
			22	6	14	2		
3	B	1	Total	C	H	O	0	0
			22	6	14	2		
3	B	1	Total	C	H	O	0	0
			22	6	14	2		
3	E	1	Total	C	H	O	0	0
			22	6	14	2		
3	E	1	Total	C	H	O	0	0
			22	6	14	2		
3	E	1	Total	C	H	O	0	0
			22	6	14	2		
3	E	1	Total	C	H	O	0	0
			22	6	14	2		

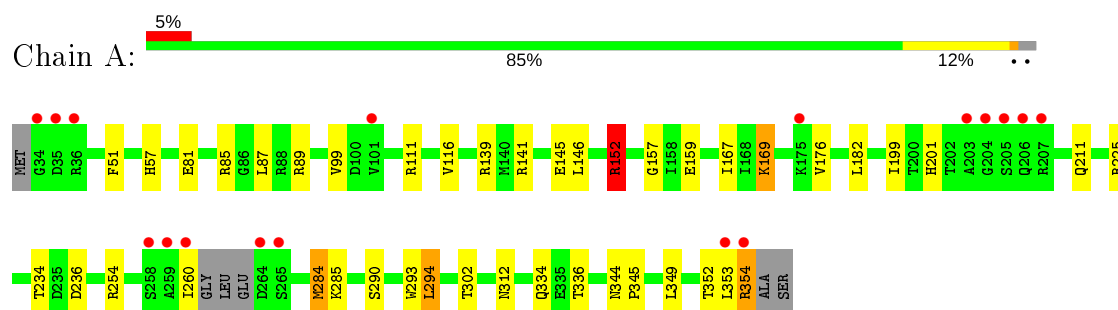
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	244	Total 244	O 244	0	0
4	G	270	Total 270	O 270	0	0
4	B	249	Total 249	O 249	0	0
4	E	266	Total 266	O 266	0	0

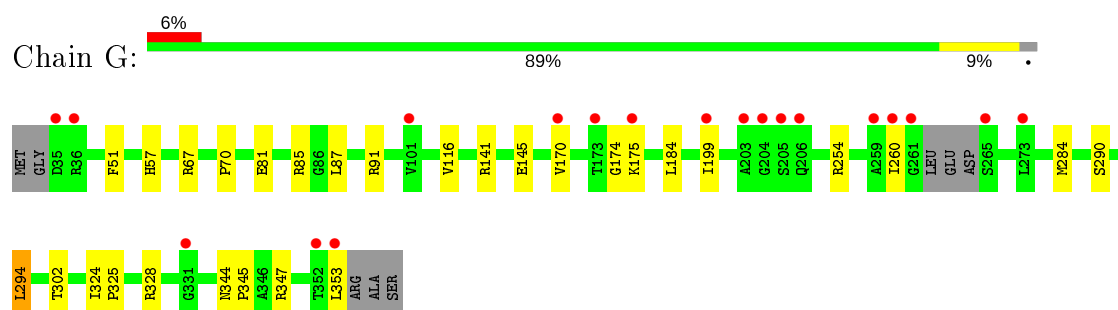
3 Residue-property plots [i](#)

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.

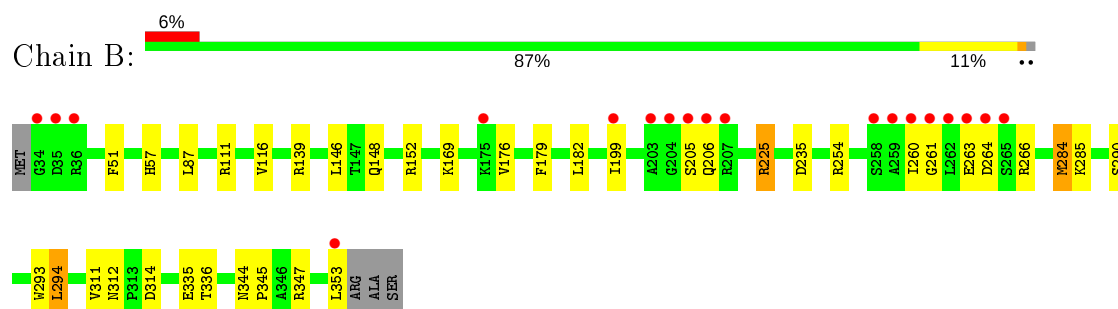
- Molecule 1: Phosphotriesterase



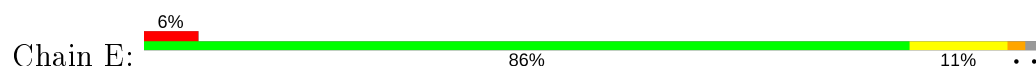
- Molecule 1: Phosphotriesterase

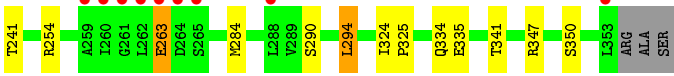
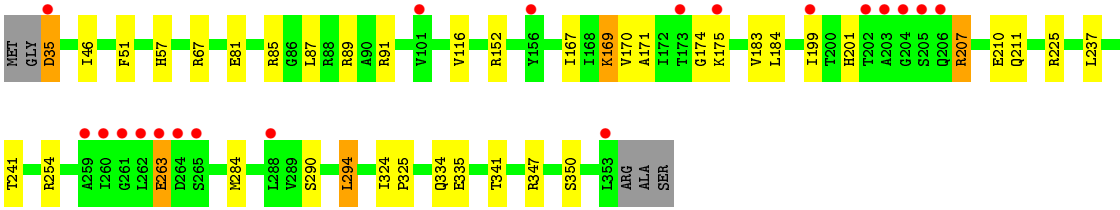


- Molecule 1: Phosphotriesterase



- Molecule 1: Phosphotriesterase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.76 Å 86.16 Å 177.67 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 1.40 29.96 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.96-1.40) 99.9 (29.96-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.40 Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.160 , 0.180 0.159 , 0.179	Depositor DCC
R_{free} test set	13059 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	22639	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7335e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ZN, MPD, KCX

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	0.59	0/2818	0.77	7/3815 (0.2%)
1	B	0.54	0/2719	0.75	2/3684 (0.1%)
1	E	0.54	0/2879	0.75	3/3899 (0.1%)
1	G	0.56	0/2743	0.77	0/3715
All	All	0.56	0/11159	0.76	12/15113 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	225	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	E	347[A]	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	E	347[B]	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	152[A]	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	152[B]	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	139	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	152[A]	ARG	CG-CD-NE	5.36	123.05	111.80
1	A	152[B]	ARG	CG-CD-NE	5.36	123.05	111.80
1	E	152	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	89	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	225	ARG	NE-CZ-NH1	-5.04	117.78	120.30

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	2643	2703	2557	43	0
1	B	2590	2652	2546	29	0
1	E	2682	2748	2544	44	1
1	G	2594	2660	2522	28	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	E	2	0	0	0	0
2	G	2	0	0	0	0
3	A	24	42	42	5	0
3	B	24	42	42	7	0
3	E	32	56	56	5	0
3	G	40	70	70	2	0
4	A	244	0	0	10	1
4	B	249	0	0	14	0
4	E	266	0	0	15	0
4	G	270	0	0	9	0
All	All	11666	10973	10379	148	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (148) 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:B:347[B]:ARG:NH1	4:B:2503:HOH:O	1.96	0.96
1:B:148[B]:GLN:OE1	4:B:2501:HOH:O	1.87	0.93
1:E:91[B]:ARG:NH1	4:E:2501:HOH:O	2.03	0.90
3:A:2403:MPD:H52	3:A:2403:MPD:H11	1.56	0.87
3:B:2403:MPD:H52	3:B:2403:MPD:H11	1.56	0.87
1:B:314:ASP:OD1	4:B:2502:HOH:O	1.93	0.85
1:G:328[B]:ARG:NH2	4:G:2502:HOH:O	2.10	0.82
3:B:2404:MPD:H52	3:B:2404:MPD:HM1	1.61	0.81
1:A:81[A]:GLU:OE2	1:A:85[A]:ARG:NE	2.19	0.75
1:G:302[B]:THR:O	4:G:2501:HOH:O	2.05	0.74
1:A:302[B]:THR:HG22	1:G:141:ARG:HH11	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:284[B]:MET:SD	4:G:2618:HOH:O	2.46	0.71
1:E:284[B]:MET:SD	4:E:2628:HOH:O	2.47	0.71
1:B:111[B]:ARG:NH1	4:B:2504:HOH:O	1.97	0.71
3:A:2403:MPD:H12	4:A:2531:HOH:O	1.90	0.71
1:A:302[B]:THR:HG21	1:G:145:GLU:OE2	1.91	0.70
3:B:2403:MPD:H12	4:B:2549:HOH:O	1.92	0.69
1:G:170[B]:VAL:HG11	1:G:184:LEU:HD12	1.74	0.68
1:E:335[A]:GLU:OE1	4:E:2502:HOH:O	2.12	0.67
1:E:210:GLU:OE1	3:E:2403:MPD:HM2	1.95	0.67
1:E:170[B]:VAL:HG11	1:E:184:LEU:HD12	1.75	0.67
1:E:335[B]:GLU:OE2	4:E:2503:HOH:O	2.12	0.66
1:A:146:LEU:HD12	1:A:182[B]:LEU:CD2	2.25	0.65
1:A:152[B]:ARG:NH1	1:A:157:GLY:O	2.29	0.65
1:G:91[B]:ARG:NE	4:G:2506:HOH:O	2.30	0.65
1:B:146:LEU:HD12	1:B:182[A]:LEU:CD2	2.26	0.65
1:E:237:LEU:O	1:E:241[A]:THR:HG23	1.97	0.65
1:B:254:ARG:HH12	3:B:2403:MPD:H51	1.63	0.63
1:E:170[B]:VAL:HG11	1:E:184:LEU:CD1	2.29	0.63
1:A:352:THR:HG22	1:A:354:ARG:HB3	1.81	0.63
1:E:254[B]:ARG:NH1	4:E:2505:HOH:O	2.23	0.63
1:B:284[B]:MET:HG3	1:B:336:THR:HG23	1.81	0.62
1:B:205:SER:H	1:B:206:GLN:HA	1.64	0.61
1:A:234[B]:THR:HG22	1:A:236:ASP:H	1.66	0.60
1:A:81[A]:GLU:OE2	1:A:85[A]:ARG:CZ	2.49	0.60
1:A:353:LEU:N	1:A:354:ARG:HA	2.16	0.60
1:E:225[A]:ARG:CD	4:E:2507:HOH:O	2.50	0.60
1:E:207:ARG:O	4:E:2504:HOH:O	2.16	0.59
1:E:211:GLN:HE22	3:E:2403:MPD:HM1	1.68	0.59
1:A:145:GLU:OE2	1:G:302[B]:THR:HG21	2.04	0.58
1:G:170[B]:VAL:HG11	1:G:184:LEU:CD1	2.34	0.57
3:E:2403:MPD:HM3	4:E:2587:HOH:O	2.03	0.57
1:E:35:ASP:N	1:E:35:ASP:OD1	2.36	0.57
1:A:99:VAL:HG11	1:A:167[B]:ILE:HD12	1.87	0.57
1:A:87:LEU:HD12	1:A:116[A]:VAL:HG12	1.86	0.56
1:A:284[B]:MET:HG3	1:A:336:THR:HG23	1.87	0.56
1:A:302[B]:THR:HG23	4:A:2642:HOH:O	2.05	0.55
1:B:87:LEU:HD12	1:B:116[A]:VAL:HG12	1.87	0.55
1:E:225[A]:ARG:HD3	4:E:2507:HOH:O	2.07	0.55
1:B:199[A]:ILE:HD11	4:B:2684:HOH:O	2.07	0.54
1:E:225[A]:ARG:HD2	4:E:2507:HOH:O	2.08	0.54
1:B:285[A]:LYS:HG2	4:B:2631:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167[A]:ILE:HD11	1:E:199[A]:ILE:HG13	1.90	0.52
1:G:254[B]:ARG:HH12	3:G:2403[B]:MPD:H51	1.75	0.52
1:A:285[A]:LYS:NZ	4:A:2502:HOH:O	2.22	0.52
1:B:225:ARG:HD3	4:B:2508:HOH:O	2.09	0.52
1:E:46:ILE:HD11	1:E:350:SER:HB2	1.92	0.51
1:B:284[A]:MET:N	1:B:284[A]:MET:SD	2.77	0.51
1:E:199[B]:ILE:HD11	4:E:2513:HOH:O	2.09	0.51
1:G:81:GLU:OE2	1:G:85:ARG:NH2	2.43	0.51
1:A:152[B]:ARG:HH21	1:G:70:PRO:HD2	1.75	0.51
1:E:167[A]:ILE:HD11	1:E:199[A]:ILE:CD1	2.41	0.51
1:E:91[B]:ARG:HD2	4:E:2581:HOH:O	2.10	0.51
1:A:146:LEU:HD12	1:A:182[B]:LEU:HD23	1.92	0.50
1:A:167[B]:ILE:HD11	1:A:349:LEU:HD21	1.92	0.50
1:B:57:HIS:HB2	1:B:294:LEU:HB3	1.94	0.50
1:E:170[B]:VAL:HG12	1:E:171[B]:ALA:H	1.76	0.50
1:E:207:ARG:N	4:E:2508:HOH:O	2.40	0.50
1:A:111[A]:ARG:NH1	4:A:2501:HOH:O	2.21	0.49
1:A:254:ARG:HH12	3:A:2403:MPD:H51	1.77	0.49
1:A:167[B]:ILE:HD11	1:A:349:LEU:CD2	2.42	0.49
1:E:170[B]:VAL:HG13	1:E:183:VAL:HG12	1.95	0.49
1:A:159:GLU:OE1	1:G:67[A]:ARG:NH2	2.45	0.49
1:B:199[A]:ILE:CD1	4:B:2684:HOH:O	2.61	0.49
1:A:57:HIS:HB2	1:A:294:LEU:HB3	1.95	0.48
1:B:205:SER:N	1:B:206:GLN:HA	2.24	0.48
1:B:199[A]:ILE:HD11	4:B:2509:HOH:O	2.13	0.47
1:B:285[B]:LYS:O	1:B:347[B]:ARG:NH2	2.47	0.47
1:B:235:ASP:OD2	1:B:266:ARG:HD3	2.15	0.47
1:B:284[A]:MET:HE3	4:B:2718:HOH:O	2.14	0.47
1:E:167[A]:ILE:CD1	1:E:199[A]:ILE:CD1	2.93	0.47
1:A:293:TRP:CH2	1:A:312:ASN:HB3	2.50	0.47
1:E:237:LEU:O	1:E:241[B]:THR:HG22	2.15	0.47
1:G:87:LEU:HD12	1:G:116:VAL:HG12	1.97	0.47
1:E:67[B]:ARG:NH2	4:E:2512:HOH:O	2.48	0.46
1:G:57:HIS:HB2	1:G:294:LEU:HB3	1.97	0.46
1:G:284[B]:MET:CE	4:G:2618:HOH:O	2.64	0.46
3:B:2403:MPD:H52	3:B:2403:MPD:C1	2.38	0.46
1:E:199[B]:ILE:HD11	4:E:2654:HOH:O	2.16	0.45
1:E:334[A]:GLN:HE22	3:E:2406:MPD:HM1	1.81	0.45
1:A:169:KCX:OQ1	1:A:201:HIS:HB2	2.17	0.45
1:A:284[A]:MET:HE3	4:A:2704:HOH:O	2.17	0.45
1:A:167[B]:ILE:HG21	1:A:199[B]:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199[A]:ILE:HD11	4:G:2694:HOH:O	2.17	0.45
1:A:141:ARG:HH11	1:G:302[B]:THR:HG22	1.81	0.44
1:E:341:THR:OG1	3:E:2406:MPD:H13	2.17	0.44
3:A:2404:MPD:O2	3:A:2404:MPD:O4	2.31	0.44
3:B:2405:MPD:H53	3:B:2405:MPD:H11	2.00	0.44
1:B:260:ILE:HG13	1:B:311:VAL:HG11	1.99	0.44
1:E:85[B]:ARG:HG2	1:E:89:ARG:NH1	2.33	0.44
1:A:199[A]:ILE:HD11	4:A:2508:HOH:O	2.18	0.44
1:B:293:TRP:CH2	1:B:312:ASN:HB3	2.52	0.44
1:G:170[B]:VAL:CG1	1:G:184:LEU:HD12	2.45	0.44
1:E:85[B]:ARG:HG2	1:E:89:ARG:HH12	1.83	0.43
1:G:57:HIS:O	1:G:294:LEU:HA	2.18	0.43
1:B:344:ASN:HB2	1:B:345:PRO:HD3	2.00	0.43
1:B:284[A]:MET:HE1	4:B:2709:HOH:O	2.18	0.43
1:E:167[A]:ILE:HD11	1:E:199[A]:ILE:CG1	2.49	0.43
1:A:285[B]:LYS:HG3	4:A:2654:HOH:O	2.18	0.43
1:E:324:ILE:HB	1:E:325[B]:PRO:HD3	2.00	0.43
1:G:344:ASN:HB2	1:G:345:PRO:HD3	2.00	0.43
1:A:57:HIS:O	1:A:294:LEU:HA	2.19	0.43
1:G:353:LEU:HA	4:G:2610:HOH:O	2.19	0.43
3:B:2405:MPD:HM2	3:B:2405:MPD:H53	2.01	0.42
1:G:199[A]:ILE:HD11	4:G:2509:HOH:O	2.18	0.42
1:A:302[B]:THR:HG22	1:G:141:ARG:NH1	2.28	0.42
1:A:199[A]:ILE:CD1	4:A:2528:HOH:O	2.67	0.42
1:A:199[A]:ILE:HD11	4:A:2528:HOH:O	2.19	0.42
1:B:57:HIS:O	1:B:294:LEU:HA	2.20	0.42
1:E:87:LEU:HD12	1:E:116[A]:VAL:HG12	2.02	0.42
1:E:169:KCX:OQ1	1:E:201:HIS:HB2	2.19	0.42
1:A:334:GLN:HE22	3:A:2404:MPD:H32	1.85	0.41
1:B:284[A]:MET:CE	4:B:2718:HOH:O	2.68	0.41
1:E:57:HIS:HB2	1:E:294:LEU:HB3	2.01	0.41
1:E:81[A]:GLU:OE2	1:E:85[A]:ARG:NH1	2.54	0.41
1:E:167[A]:ILE:HD11	1:E:199[A]:ILE:HD11	2.02	0.41
1:G:67[B]:ARG:NH2	4:G:2513:HOH:O	2.54	0.41
1:G:324:ILE:HB	1:G:325:PRO:HD3	2.01	0.41
1:A:234[B]:THR:CG2	1:A:236:ASP:H	2.31	0.41
1:A:344:ASN:HB2	1:A:345:PRO:HD3	2.01	0.41
1:B:347[B]:ARG:NH1	4:B:2514:HOH:O	2.52	0.41
1:E:167[B]:ILE:HD13	1:E:199[B]:ILE:HG22	2.02	0.41
1:E:57:HIS:O	1:E:294:LEU:HA	2.20	0.41
1:B:139:ARG:HA	1:B:179:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81[A]:GLU:HG2	1:E:85[A]:ARG:NH1	2.36	0.41
1:E:170[B]:VAL:HG13	1:E:183:VAL:CG1	2.51	0.41
1:A:285[B]:LYS:CE	4:A:2654:HOH:O	2.70	0.40
1:B:335:GLU:H	1:B:335:GLU:CD	2.23	0.40
1:E:324:ILE:HB	1:E:325[A]:PRO:HD3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335[A]:GLU:OE1	4:A:2654:HOH:O[4_455]	2.18	0.02

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	353/324 (109%)	344 (98%)	8 (2%)	1 (0%)	41	18
1	B	344/324 (106%)	330 (96%)	10 (3%)	4 (1%)	13	1
1	E	364/324 (112%)	349 (96%)	12 (3%)	3 (1%)	19	4
1	G	345/324 (106%)	334 (97%)	9 (3%)	2 (1%)	25	7
All	All	1406/1296 (108%)	1357 (96%)	39 (3%)	10 (1%)	19	5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	GLU
1	E	174	GLY
1	E	207	ARG
1	G	174	GLY
1	B	264	ASP

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Mol	Chain	Res	Type
1	E	263	GLU
1	G	260	ILE
1	B	176	VAL
1	A	176	VAL
1	B	261	GLY

5.3.2 Protein sidechains ⓘ

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	296/263 (112%)	286 (97%)	10 (3%)	37	8
1	B	285/263 (108%)	276 (97%)	9 (3%)	39	9
1	E	299/263 (114%)	293 (98%)	6 (2%)	55	23
1	G	283/263 (108%)	279 (99%)	4 (1%)	67	40
All	All	1163/1052 (111%)	1134 (98%)	29 (2%)	52	14

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

Mol	Chain	Res	Type
1	A	51	PHE
1	A	152[A]	ARG
1	A	152[B]	ARG
1	A	211[A]	GLN
1	A	211[B]	GLN
1	A	284[A]	MET
1	A	284[B]	MET
1	A	290	SER
1	A	294	LEU
1	A	354	ARG
1	G	51	PHE
1	G	175	LYS
1	G	290	SER
1	G	294	LEU
1	B	51	PHE
1	B	152[A]	ARG

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Mol	Chain	Res	Type
1	B	152[B]	ARG
1	B	284[A]	MET
1	B	284[B]	MET
1	B	284[C]	MET
1	B	290	SER
1	B	294	LEU
1	B	353	LEU
1	E	35	ASP
1	E	51	PHE
1	E	175	LYS
1	E	263	GLU
1	E	290	SER
1	E	294	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	KCX	A	169	1,2	7,11,12	0.54	0	4,12,14	1.53	1 (25%)
1	KCX	G	169	1,2	7,11,12	0.58	0	4,12,14	1.18	0
1	KCX	B	169	1,2	7,11,12	0.57	0	4,12,14	1.52	1 (25%)
1	KCX	E	169	1,2	7,11,12	0.76	0	4,12,14	1.73	1 (25%)

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
1	KCX	A	169	1,2	-	0/7/10/12	-
1	KCX	G	169	1,2	-	0/7/10/12	-
1	KCX	B	169	1,2	-	0/7/10/12	-
1	KCX	E	169	1,2	-	0/7/10/12	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	169	KCX	CE-NZ-CX	-2.90	118.03	122.95
1	B	169	KCX	CE-NZ-CX	-2.81	118.19	122.95
1	A	169	KCX	CE-NZ-CX	-2.73	118.33	122.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	169	KCX	1	0
1	E	169	KCX	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 8 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MPD	G	2403[B]	-	7,7,7	0.53	0	9,10,10	0.59	0
3	MPD	G	2403[A]	-	7,7,7	0.60	0	9,10,10	0.66	0
3	MPD	E	2403	-	7,7,7	0.71	0	9,10,10	0.55	0
3	MPD	B	2403	-	7,7,7	0.54	0	9,10,10	0.65	0
3	MPD	A	2403	-	7,7,7	0.65	0	9,10,10	0.61	0
3	MPD	E	2406	-	7,7,7	0.60	0	9,10,10	0.86	0
3	MPD	B	2404	-	7,7,7	0.69	0	9,10,10	0.72	0
3	MPD	G	2406	-	7,7,7	0.67	0	9,10,10	0.46	0
3	MPD	A	2405	-	7,7,7	0.73	0	9,10,10	0.38	0
3	MPD	B	2405	-	7,7,7	0.63	0	9,10,10	0.46	0
3	MPD	E	2405	-	7,7,7	0.73	0	9,10,10	0.53	0
3	MPD	G	2405	-	7,7,7	0.64	0	9,10,10	0.50	0
3	MPD	A	2404	-	7,7,7	0.58	0	9,10,10	0.36	0
3	MPD	G	2404	-	7,7,7	0.60	0	9,10,10	0.39	0
3	MPD	E	2404	-	7,7,7	0.48	0	9,10,10	0.73	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
3	MPD	G	2403[B]	-	-	2/5/5/5	-
3	MPD	G	2403[A]	-	-	0/5/5/5	-
3	MPD	E	2403	-	-	1/5/5/5	-
3	MPD	B	2403	-	-	3/5/5/5	-
3	MPD	A	2403	-	-	4/5/5/5	-
3	MPD	E	2406	-	-	0/5/5/5	-
3	MPD	B	2404	-	-	4/5/5/5	-
3	MPD	G	2406	-	-	2/5/5/5	-
3	MPD	A	2405	-	-	0/5/5/5	-
3	MPD	B	2405	-	-	2/5/5/5	-
3	MPD	E	2405	-	-	2/5/5/5	-
3	MPD	G	2405	-	-	3/5/5/5	-
3	MPD	A	2404	-	-	0/5/5/5	-
3	MPD	G	2404	-	-	0/5/5/5	-
3	MPD	E	2404	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2403	MPD	C1-C2-C3-C4
3	B	2403	MPD	O2-C2-C3-C4
3	B	2404	MPD	O2-C2-C3-C4
3	B	2404	MPD	CM-C2-C3-C4
3	A	2403	MPD	C1-C2-C3-C4
3	A	2403	MPD	O2-C2-C3-C4
3	G	2405	MPD	C1-C2-C3-C4
3	G	2406	MPD	C2-C3-C4-O4
3	G	2406	MPD	C2-C3-C4-C5
3	E	2405	MPD	C1-C2-C3-C4
3	E	2405	MPD	O2-C2-C3-C4
3	G	2405	MPD	O2-C2-C3-C4
3	A	2403	MPD	C2-C3-C4-C5
3	G	2403[B]	MPD	C2-C3-C4-C5
3	B	2404	MPD	C1-C2-C3-C4
3	E	2403	MPD	CM-C2-C3-C4
3	A	2403	MPD	CM-C2-C3-C4
3	G	2405	MPD	CM-C2-C3-C4
3	G	2403[B]	MPD	C1-C2-C3-C4
3	B	2405	MPD	O2-C2-C3-C4
3	B	2403	MPD	C2-C3-C4-C5
3	B	2404	MPD	C2-C3-C4-C5
3	B	2405	MPD	C2-C3-C4-C5

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2403[B]	MPD	1	0
3	E	2403	MPD	3	0
3	B	2403	MPD	4	0
3	A	2403	MPD	3	0
3	E	2406	MPD	2	0
3	B	2404	MPD	1	0
3	G	2406	MPD	1	0
3	B	2405	MPD	2	0
3	A	2404	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, 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	317/324 (97%)	-0.05	17 (5%) 25 24	15, 20, 38, 80	0
1	B	319/324 (98%)	0.11	19 (5%) 21 20	15, 21, 42, 89	0
1	E	318/324 (98%)	0.02	20 (6%) 20 18	16, 21, 45, 84	0
1	G	315/324 (97%)	-0.05	19 (6%) 21 20	16, 22, 38, 74	0
All	All	1269/1296 (97%)	0.01	75 (5%) 22 20	15, 21, 40, 89	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	262	LEU	18.2
1	B	262	LEU	15.0
1	A	260	ILE	10.7
1	B	261	GLY	10.1
1	B	205	SER	9.7
1	B	263	GLU	9.3
1	B	260	ILE	9.0
1	A	205	SER	8.5
1	E	204	GLY	7.2
1	B	204	GLY	6.4
1	E	261	GLY	6.2
1	G	204	GLY	6.0
1	E	263	GLU	5.9
1	A	259[A]	ALA	5.5
1	G	259	ALA	5.4
1	A	34	GLY	5.3
1	B	206	GLN	5.2
1	B	259[A]	ALA	5.1
1	B	34	GLY	5.1
1	A	203	ALA	4.9
1	G	203	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	264	ASP	4.7
1	A	353	LEU	4.6
1	G	353	LEU	4.6
1	B	353	LEU	4.5
1	E	203	ALA	4.4
1	G	261	GLY	4.4
1	E	205	SER	4.3
1	E	353	LEU	4.2
1	A	206	GLN	4.2
1	B	175	LYS	4.1
1	G	175	LYS	3.8
1	G	260	ILE	3.8
1	E	265	SER	3.8
1	E	264	ASP	3.6
1	B	264	ASP	3.5
1	B	203	ALA	3.4
1	E	175	LYS	3.4
1	E	202	THR	3.3
1	G	36	ARG	3.3
1	E	259[A]	ALA	3.2
1	A	175	LYS	3.2
1	B	35	ASP	3.1
1	E	199[A]	ILE	3.1
1	G	35	ASP	3.0
1	E	35	ASP	3.0
1	E	288	LEU	2.8
1	A	258[A]	SER	2.8
1	A	35	ASP	2.8
1	B	258[A]	SER	2.8
1	A	204	GLY	2.8
1	G	199[A]	ILE	2.7
1	B	265	SER	2.7
1	A	354	ARG	2.7
1	A	265	SER	2.7
1	E	173	THR	2.6
1	G	101	VAL	2.6
1	B	207	ARG	2.5
1	G	273	LEU	2.5
1	G	170[A]	VAL	2.5
1	G	205	SER	2.4
1	G	265	SER	2.4
1	E	260	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	156[A]	TYR	2.3
1	B	36	ARG	2.3
1	B	199[A]	ILE	2.2
1	E	206	GLN	2.2
1	A	101	VAL	2.1
1	A	207	ARG	2.1
1	A	36	ARG	2.1
1	G	206	GLN	2.1
1	G	331	GLY	2.1
1	G	173	THR	2.1
1	E	101	VAL	2.0
1	G	352	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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
1	KCX	A	169	12/13	0.97	0.11	15,18,24,25	0
1	KCX	B	169	12/13	0.97	0.12	15,19,24,24	0
1	KCX	E	169	12/13	0.97	0.12	16,19,23,26	0
1	KCX	G	169	12/13	0.98	0.15	16,19,25,25	0

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, 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
3	MPD	E	2406	8/8	0.47	0.36	61,74,77,78	0
3	MPD	A	2404	8/8	0.51	0.30	59,71,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MPD	E	2405	8/8	0.62	0.35	65,78,81,84	0
3	MPD	A	2405	8/8	0.71	0.25	62,74,77,78	0
3	MPD	G	2406	8/8	0.80	0.25	64,76,80,82	0
3	MPD	B	2404	8/8	0.81	0.19	54,65,72,72	0
3	MPD	E	2403	8/8	0.82	0.25	30,46,53,57	0
3	MPD	A	2403	8/8	0.83	0.12	24,38,45,50	0
3	MPD	B	2405	8/8	0.83	0.17	64,77,80,80	0
3	MPD	B	2403	8/8	0.83	0.14	27,40,45,52	0
3	MPD	G	2405	8/8	0.85	0.20	34,48,56,59	0
3	MPD	G	2404	8/8	0.86	0.20	40,48,54,55	0
3	MPD	E	2404	8/8	0.86	0.10	29,38,45,45	0
3	MPD	G	2403[B]	8/8	0.94	0.10	24,30,34,34	22
3	MPD	G	2403[A]	8/8	0.94	0.10	23,28,33,33	22
2	ZN	B	2401	1/1	0.99	0.07	16,16,16,16	0
2	ZN	E	2402	1/1	0.99	0.04	23,23,23,23	0
2	ZN	A	2401	1/1	0.99	0.06	16,16,16,16	0
2	ZN	E	2401	1/1	0.99	0.05	19,19,19,19	0
2	ZN	G	2402	1/1	1.00	0.06	21,21,21,21	0
2	ZN	A	2402	1/1	1.00	0.04	18,18,18,18	0
2	ZN	B	2402	1/1	1.00	0.07	18,18,18,18	0
2	ZN	G	2401	1/1	1.00	0.05	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.