



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:08 AM GMT

PDB ID : 3KRA
Title : Mint heterotetrameric geranyl pyrophosphate synthase in complex with magnesium
Authors : Chang, T.-H.; Ko, T.-P.; Hsieh, F.-L.; Wang, A.H.-J.
Deposited on : 2009-11-18
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

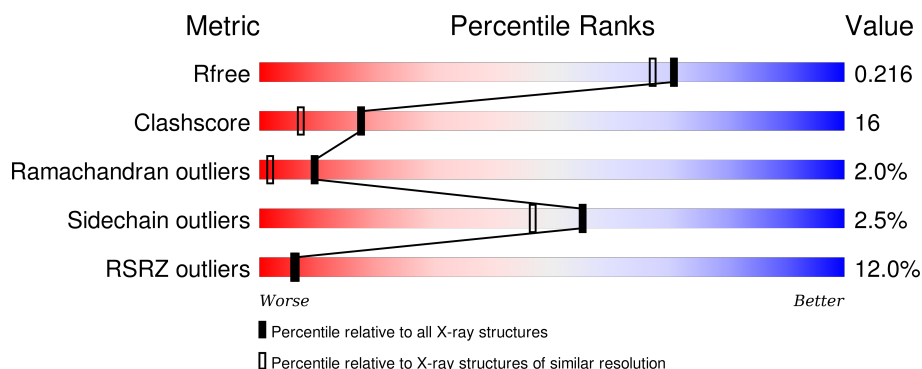
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	295	<div> <div>5%</div> <div>83%</div> <div>9%</div> <div>5%</div> </div>
1	D	295	<div> <div>17%</div> <div>64%</div> <div>26%</div> <div>6%</div> </div>
2	B	274	<div> <div>13%</div> <div>77%</div> <div>16%</div> <div>5%</div> </div>
2	C	274	<div> <div>12%</div> <div>73%</div> <div>23%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	C	2001	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9540 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 Geranyl diphosphate synthase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2120	1338	372	392	18			
1	D	277	Total	C	N	O	S	0	0	0
			2102	1326	368	390	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q9SBR3
D	1	MET	-	EXPRESSION TAG	UNP Q9SBR3

- Molecule 2 is a protein called Geranyl diphosphate synthase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	0	0	0
			1954	1233	339	368	14			
2	C	271	Total	C	N	O	S	0	0	0
			2056	1297	361	384	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	EXPRESSION TAG	UNP Q9SBR4
B	267	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	268	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	269	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	270	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	271	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	272	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	273	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	274	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	1	MET	-	EXPRESSION TAG	UNP Q9SBR4

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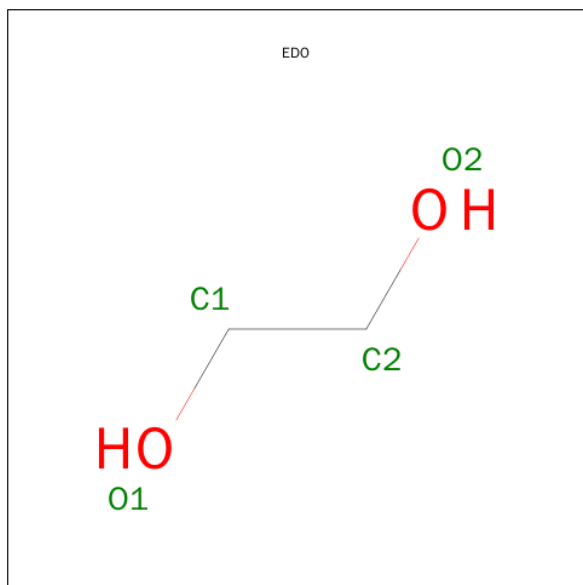
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Chain	Residue	Modelled	Actual	Comment	Reference
C	267	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	268	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	269	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	270	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	271	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	272	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	273	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	274	HIS	-	EXPRESSION TAG	UNP Q9SBR4

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



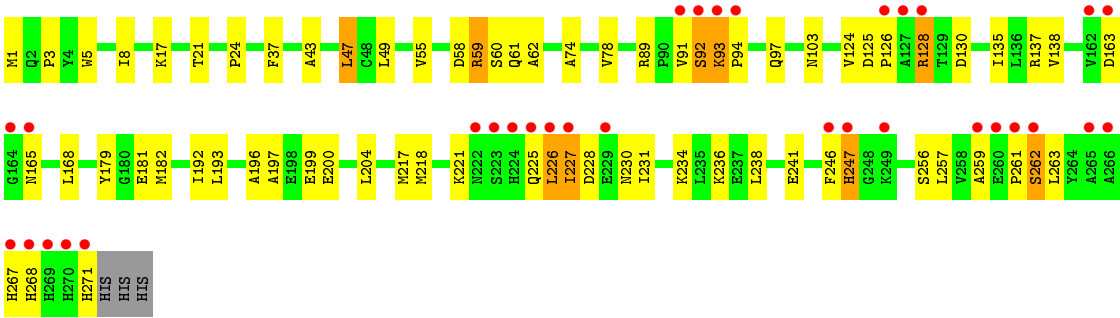
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	383	Total 383	O 383	0	0
5	B	319	Total 319	O 319	0	0
5	C	287	Total 287	O 287	0	0
5	D	312	Total 312	O 312	0	0

- Molecule 1: Geranyl diphosphate synthase large subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.28Å 109.25Å 182.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.84 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (30.00-1.90) 93.2 (29.84-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.176 , 0.216 0.176 , 0.216	Depositor DCC
R_{free} test set	4057 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 80929 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9540	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EDO

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	0.97	0/2155	0.87	1/2903 (0.0%)
1	D	0.88	1/2137 (0.0%)	0.85	3/2881 (0.1%)
2	B	0.81	0/1993	0.83	1/2695 (0.0%)
2	C	0.82	1/2102 (0.0%)	0.80	2/2845 (0.1%)
All	All	0.87	2/8387 (0.0%)	0.84	7/11324 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	138	VAL	CB-CG2	5.42	1.64	1.52
1	D	189	VAL	CB-CG1	-5.06	1.42	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	LYS	C-N-CD	5.73	140.44	128.40
1	D	286	LEU	CA-CB-CG	-5.71	102.16	115.30
1	A	45	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	61	ASP	CB-CG-OD2	-5.34	113.49	118.30
2	C	182	MET	CG-SD-CE	5.31	108.70	100.20
2	C	47	LEU	CA-CB-CG	5.25	127.37	115.30
1	D	47	ARG	NE-CZ-NH2	5.04	122.82	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	2120	0	2146	35	0
1	D	2102	0	2120	88	0
2	B	1954	0	1948	75	0
2	C	2056	0	2031	69	0
3	A	2	0	0	0	0
3	D	1	0	0	0	0
4	C	4	0	6	0	0
5	A	383	0	0	10	1
5	B	319	0	0	8	0
5	C	287	0	0	13	1
5	D	312	0	0	10	1
All	All	9540	0	8251	266	2

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 16.

All (266) 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:A:138:ARG:HD2	5:A:862:HOH:O	1.39	1.20
2:B:200:GLU:HG3	5:B:890:HOH:O	1.46	1.16
1:D:286:LEU:HD13	5:D:1297:HOH:O	1.46	1.11
2:C:236:LYS:HD2	5:C:1191:HOH:O	1.53	1.07
2:B:54:LEU:HG	2:B:250:ASN:HB3	1.41	0.99
2:C:125:ASP:HB3	2:C:128:ARG:HG3	1.49	0.92
2:B:54:LEU:HG	2:B:250:ASN:CB	2.01	0.90
2:B:1:MET:HE2	2:B:3:PRO:HG2	1.51	0.90
2:B:249:LYS:O	2:B:253:LEU:N	2.04	0.90
2:B:93:LYS:HB3	2:B:94:PRO:HD3	1.52	0.90
1:D:211:ASN:HB3	5:D:942:HOH:O	1.73	0.88
2:C:58:ASP:O	2:C:61:GLN:HG2	1.77	0.84
2:C:58:ASP:OD2	2:C:60:SER:HB3	1.79	0.82
1:D:222:ASP:O	1:D:226:VAL:HG22	1.80	0.81
2:C:230:ASN:O	2:C:234:LYS:HG3	1.78	0.81
2:B:17:LYS:HE3	5:B:1044:HOH:O	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:262:SER:O	2:C:263:LEU:HD23	1.83	0.79
2:B:249:LYS:HG3	2:B:253:LEU:HB3	1.64	0.79
1:D:216:LEU:C	1:D:218:GLN:H	1.85	0.79
1:A:227:THR:O	5:A:1255:HOH:O	2.00	0.79
1:D:279:ARG:HH11	1:D:279:ARG:HB3	1.45	0.79
2:B:250:ASN:HA	2:B:253:LEU:HG	1.64	0.79
2:B:1:MET:CE	2:B:3:PRO:HG2	2.11	0.78
2:C:179:TYR:OH	5:C:1036:HOH:O	2.03	0.77
1:A:227:THR:HB	1:A:228:LYS:HD2	1.66	0.76
1:D:279:ARG:HH11	1:D:279:ARG:CB	1.97	0.76
1:A:165:MET:CG	1:A:166:ALA:H	1.99	0.75
1:D:221:ASP:HA	1:D:224:LEU:HB2	1.68	0.75
1:D:279:ARG:HH11	1:D:279:ARG:CG	1.99	0.75
2:C:221:LYS:HE2	2:C:227:ILE:HG21	1.68	0.75
2:B:93:LYS:HB3	2:B:94:PRO:CD	2.17	0.74
2:C:43:ALA:O	2:C:47:LEU:HB2	1.88	0.74
2:C:268:HIS:O	2:C:271:HIS:HB3	1.87	0.74
1:D:186:GLN:HE21	1:D:211:ASN:HD21	1.36	0.73
1:D:292:TYR:CD2	5:D:1304:HOH:O	2.41	0.72
1:A:165:MET:HG2	1:A:166:ALA:H	1.55	0.71
1:A:228:LYS:HD2	1:A:228:LYS:H	1.55	0.71
2:C:125:ASP:CB	2:C:128:ARG:HG3	2.21	0.70
1:D:44:LYS:HG3	5:D:724:HOH:O	1.91	0.70
2:B:249:LYS:HE2	2:B:253:LEU:HA	1.74	0.69
1:D:8:MET:SD	1:D:49:MET:SD	2.90	0.68
1:D:292:TYR:CE2	5:D:1304:HOH:O	2.47	0.68
2:B:54:LEU:HG	2:B:250:ASN:ND2	2.08	0.68
1:D:218:GLN:HA	1:D:221:ASP:HB3	1.74	0.68
2:B:214:LEU:HG	2:B:218:MET:HE3	1.74	0.68
1:A:208:LYS:HE3	5:A:912:HOH:O	1.94	0.67
2:B:252:GLU:HA	2:B:255:SER:OG	1.95	0.67
2:C:221:LYS:HE2	2:C:227:ILE:HG12	1.75	0.67
1:D:246:THR:N	1:D:250:LYS:HD2	2.10	0.67
1:D:256:LYS:HB3	5:D:378:HOH:O	1.93	0.66
1:D:202:GLU:OE2	5:D:1230:HOH:O	2.14	0.66
2:B:229:GLU:HA	2:B:232:ILE:HD12	1.75	0.66
2:C:55:VAL:O	5:C:1157:HOH:O	2.14	0.65
2:B:218:MET:HA	2:B:221:LYS:HG3	1.79	0.65
2:C:49:LEU:HD13	2:C:59:ARG:HD3	1.78	0.65
1:D:254:VAL:HA	1:D:257:SER:HB2	1.79	0.64
2:C:221:LYS:CE	2:C:227:ILE:HG21	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LEU:CG	2:B:250:ASN:HB3	2.24	0.64
2:B:228:ASP:OD2	2:B:230:ASN:HB2	1.97	0.63
1:D:222:ASP:C	1:D:224:LEU:H	2.02	0.63
2:B:250:ASN:HA	2:B:253:LEU:CG	2.29	0.62
2:B:253:LEU:HD11	2:B:254:MET:HE1	1.82	0.62
1:A:95:ARG:HH11	1:A:95:ARG:HG2	1.64	0.62
1:D:217:PHE:HA	1:D:293:ARG:HH11	1.66	0.61
2:C:97:GLN:NE2	5:C:326:HOH:O	2.33	0.61
2:C:267:HIS:CD2	2:C:267:HIS:H	2.19	0.60
2:B:54:LEU:HG	2:B:250:ASN:CG	2.21	0.60
1:D:221:ASP:O	1:D:225:ASP:N	2.35	0.60
2:C:217:MET:CE	2:C:231:ILE:HG21	2.32	0.60
2:B:93:LYS:CB	2:B:94:PRO:HD3	2.27	0.60
2:C:234:LYS:NZ	5:C:332:HOH:O	2.35	0.60
1:D:216:LEU:C	1:D:218:GLN:N	2.54	0.60
2:B:171:ILE:HG22	2:B:217:MET:CE	2.32	0.60
2:C:221:LYS:NZ	2:C:227:ILE:HG21	2.18	0.59
1:D:289:TYR:O	1:D:291:ALA:N	2.36	0.59
1:A:165:MET:CG	1:A:166:ALA:N	2.66	0.59
1:D:8:MET:HE3	1:D:49:MET:HE1	1.85	0.59
2:C:8:ILE:HG23	2:C:49:LEU:HD12	1.85	0.59
2:C:168:LEU:HB3	2:C:231:ILE:HD11	1.83	0.59
2:C:246:PHE:O	2:C:247:HIS:O	2.21	0.59
2:C:137:ARG:HD3	2:C:192:ILE:HD13	1.84	0.58
2:B:214:LEU:HG	2:B:218:MET:CE	2.32	0.58
2:B:163:ASP:HA	2:B:224:HIS:CE1	2.38	0.58
1:D:279:ARG:NH1	1:D:279:ARG:CG	2.62	0.58
1:D:216:LEU:O	1:D:218:GLN:N	2.37	0.58
1:D:248:TYR:O	1:D:252:ILE:HG12	2.04	0.57
2:C:267:HIS:N	2:C:267:HIS:CD2	2.70	0.57
1:D:253:GLY:O	1:D:255:GLU:N	2.36	0.57
1:A:221:ASP:HB3	5:A:917:HOH:O	2.03	0.57
2:B:253:LEU:HD12	2:B:253:LEU:C	2.24	0.57
2:B:250:ASN:ND2	2:B:253:LEU:HD21	2.19	0.57
1:D:252:ILE:HD12	1:D:256:LYS:O	2.04	0.57
2:C:221:LYS:HB2	2:C:227:ILE:HB	1.87	0.56
2:C:217:MET:HE2	2:C:231:ILE:HG21	1.86	0.56
2:C:21:THR:HG22	5:C:378:HOH:O	2.05	0.56
2:B:2:GLN:H	2:B:3:PRO:HD2	1.70	0.56
2:B:250:ASN:C	2:B:252:GLU:N	2.58	0.56
2:C:227:ILE:HG23	2:C:227:ILE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:GLN:NE2	1:D:211:ASN:HD21	2.01	0.56
1:D:279:ARG:HG2	1:D:279:ARG:NH1	2.21	0.56
1:A:228:LYS:HD2	1:A:228:LYS:N	2.21	0.55
2:B:221:LYS:HB3	2:B:227:ILE:HD11	1.88	0.55
2:C:55:VAL:HG11	2:C:196:ALA:HB2	1.89	0.55
1:D:223:ILE:HD13	1:D:258:LYS:HG3	1.88	0.54
1:D:160:VAL:O	1:D:163:GLU:HG3	2.06	0.54
1:D:292:TYR:HD2	5:D:1304:HOH:O	1.85	0.54
2:B:228:ASP:O	2:B:232:ILE:HG13	2.06	0.54
2:B:250:ASN:C	2:B:252:GLU:H	2.10	0.54
1:D:176:ILE:O	1:D:180:LYS:HG2	2.07	0.54
1:D:168:VAL:O	1:D:168:VAL:HG23	2.07	0.54
2:B:236:LYS:NZ	5:B:1112:HOH:O	2.40	0.54
1:D:8:MET:CE	1:D:49:MET:CE	2.86	0.54
1:D:186:GLN:HA	1:D:210:ALA:CB	2.38	0.54
1:D:50:LEU:CD2	1:D:286:LEU:HD22	2.38	0.54
2:B:249:LYS:O	2:B:253:LEU:HB3	2.07	0.54
2:B:221:LYS:HB3	2:B:227:ILE:CD1	2.38	0.54
2:B:226:LEU:O	2:B:228:ASP:N	2.41	0.53
1:A:166:ALA:C	1:A:168:VAL:H	2.11	0.53
2:C:218:MET:HA	2:C:221:LYS:HD2	1.90	0.53
1:A:165:MET:HG2	1:A:166:ALA:N	2.21	0.53
2:B:253:LEU:HD11	2:B:254:MET:CE	2.38	0.53
1:D:253:GLY:C	1:D:255:GLU:H	2.12	0.53
1:D:50:LEU:HD21	1:D:286:LEU:CD2	2.39	0.53
1:D:68:ALA:HA	1:D:124:VAL:HG22	1.90	0.53
2:B:131:ASP:O	2:B:135:ILE:HG12	2.09	0.53
2:B:54:LEU:O	2:B:54:LEU:HD23	2.08	0.52
2:B:237:GLU:O	2:B:241:GLU:HB2	2.09	0.52
2:C:168:LEU:HD22	2:C:231:ILE:HD12	1.91	0.52
2:B:249:LYS:HE2	2:B:253:LEU:CA	2.39	0.52
1:D:213:ILE:HD12	1:D:290:ILE:CD1	2.40	0.52
2:B:1:MET:CG	2:B:2:GLN:N	2.72	0.52
1:D:187:GLY:O	1:D:191:LEU:HG	2.10	0.52
1:A:162:SER:C	1:A:164:GLY:H	2.13	0.51
1:A:165:MET:HG2	1:A:167:GLU:H	1.75	0.51
1:A:83:ASP:O	1:A:89:ASP:HB2	2.10	0.51
2:C:256:SER:HB2	2:C:261:PRO:HD3	1.92	0.51
2:B:233:GLY:O	2:B:236:LYS:HG2	2.10	0.51
1:D:249:PRO:O	1:D:253:GLY:HA2	2.11	0.51
2:B:224:HIS:O	2:B:226:LEU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:HD12	1:D:214:GLY:HA2	1.92	0.51
2:B:54:LEU:HG	2:B:250:ASN:HD22	1.76	0.51
2:C:218:MET:O	2:C:221:LYS:HG2	2.11	0.50
2:B:54:LEU:HD12	2:B:254:MET:HE3	1.93	0.50
2:C:238:LEU:HD22	5:C:773:HOH:O	2.09	0.50
1:D:44:LYS:HE3	5:D:724:HOH:O	2.11	0.50
1:D:219:VAL:HG21	1:D:260:PHE:CD2	2.46	0.50
1:D:158:VAL:HG12	1:D:176:ILE:HD11	1.92	0.50
2:C:17:LYS:HG3	2:C:37:PHE:CZ	2.47	0.50
1:D:139:VAL:HG21	1:D:195:LEU:HG	1.93	0.49
1:D:246:THR:N	1:D:250:LYS:CD	2.74	0.49
2:B:171:ILE:HG22	2:B:217:MET:HE3	1.94	0.49
1:D:71:ALA:HB2	1:D:124:VAL:HG23	1.94	0.49
1:A:228:LYS:CD	1:A:228:LYS:H	2.25	0.49
1:D:253:GLY:C	1:D:255:GLU:N	2.66	0.49
2:B:210:TYR:CE2	2:B:238:LEU:HD13	2.48	0.49
2:C:91:VAL:O	2:C:92:SER:C	2.50	0.49
1:A:276:HIS:HD2	1:A:279:ARG:CZ	2.26	0.49
2:B:1:MET:HE2	2:B:3:PRO:CG	2.34	0.49
1:D:223:ILE:O	1:D:223:ILE:HG22	2.13	0.49
1:D:223:ILE:HG21	1:D:258:LYS:HE3	1.95	0.49
2:C:24:PRO:HD2	5:C:1132:HOH:O	2.11	0.49
1:D:57:LEU:HD22	1:D:283:LEU:HD12	1.95	0.48
1:D:49:MET:HB3	5:D:1297:HOH:O	2.12	0.48
1:D:286:LEU:O	1:D:286:LEU:HG	2.13	0.48
1:D:149:SER:O	1:D:154:ALA:HB2	2.14	0.48
1:A:166:ALA:O	1:A:168:VAL:N	2.46	0.48
2:B:54:LEU:HA	2:B:250:ASN:ND2	2.29	0.47
2:C:196:ALA:HB1	2:C:200:GLU:HB2	1.95	0.47
2:C:238:LEU:CD2	5:C:773:HOH:O	2.62	0.47
2:B:8:ILE:HG23	2:B:49:LEU:HD12	1.94	0.47
1:D:189:VAL:CG1	1:D:206:LEU:HB3	2.45	0.47
1:D:186:GLN:HE21	1:D:211:ASN:ND2	2.09	0.47
1:D:247:THR:O	1:D:251:LEU:HG	2.14	0.47
1:A:138:ARG:HB2	5:A:862:HOH:O	2.14	0.47
2:B:252:GLU:O	2:B:255:SER:HB2	2.15	0.47
2:B:93:LYS:CB	2:B:94:PRO:CD	2.89	0.47
1:D:224:LEU:HD22	1:D:294:ASP:HA	1.97	0.47
1:A:95:ARG:HD2	1:A:95:ARG:N	2.29	0.47
2:C:103:ASN:HB3	1:D:87:CYS:O	2.14	0.47
1:D:248:TYR:HB2	1:D:249:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:MET:HE2	2:C:5:TRP:CB	2.45	0.46
2:B:226:LEU:HD12	5:B:1105:HOH:O	2.15	0.46
2:C:74:ALA:O	2:C:78:VAL:HG23	2.16	0.46
2:B:247:HIS:ND1	5:B:1272:HOH:O	2.36	0.46
2:C:221:LYS:HE2	2:C:227:ILE:CG1	2.44	0.46
1:D:128:THR:O	1:D:129:LYS:HD3	2.16	0.46
2:C:47:LEU:HD13	2:C:257:LEU:CD2	2.46	0.46
2:B:233:GLY:HA2	2:B:236:LYS:HG2	1.98	0.46
2:C:256:SER:HA	2:C:259:ALA:O	2.15	0.46
2:B:252:GLU:HG2	2:B:252:GLU:O	2.16	0.46
2:C:62:ALA:HA	2:C:193:LEU:HD13	1.97	0.46
1:A:177:HIS:HD2	1:A:248:TYR:OH	1.99	0.46
2:B:1:MET:SD	5:B:1263:HOH:O	2.61	0.45
2:C:228:ASP:CG	2:C:230:ASN:HD22	2.20	0.45
2:C:204:LEU:HD23	2:C:204:LEU:HA	1.76	0.45
2:C:226:LEU:O	2:C:228:ASP:N	2.49	0.45
2:C:181:GLU:HA	2:C:181:GLU:OE2	2.16	0.45
1:A:227:THR:CB	1:A:228:LYS:HD2	2.43	0.45
2:C:5:TRP:CZ2	2:C:257:LEU:HB2	2.52	0.45
2:C:89:ARG:NH1	5:C:1034:HOH:O	2.48	0.45
1:D:223:ILE:HD13	1:D:258:LYS:CG	2.47	0.44
2:C:92:SER:O	2:C:94:PRO:N	2.49	0.44
1:A:177:HIS:HE1	5:A:833:HOH:O	1.98	0.44
1:A:217:PHE:CE2	1:A:221:ASP:OD1	2.71	0.44
2:B:218:MET:HA	2:B:221:LYS:CD	2.47	0.44
2:C:3:PRO:HG2	5:C:1129:HOH:O	2.17	0.44
2:C:197:ALA:HB1	2:C:199:GLU:OE2	2.17	0.44
1:D:46:VAL:HA	1:D:49:MET:HE2	2.00	0.43
2:B:206:ASN:HB3	2:B:242:GLU:HG3	2.00	0.43
1:A:138:ARG:NH2	5:A:584:HOH:O	2.45	0.43
2:C:124:VAL:HG22	2:C:135:ILE:HD12	2.00	0.43
1:D:50:LEU:CD2	1:D:286:LEU:CD2	2.96	0.43
2:B:210:TYR:CE1	2:B:238:LEU:HB3	2.53	0.43
1:A:57:LEU:HD12	1:A:279:ARG:HB3	2.01	0.43
2:B:250:ASN:ND2	2:B:253:LEU:CD2	2.80	0.43
2:C:93:LYS:HB3	2:C:94:PRO:HD3	2.01	0.43
1:D:66:MET:HB3	1:D:67:PRO:HD3	2.01	0.43
2:C:221:LYS:HE2	2:C:227:ILE:CG2	2.42	0.43
1:D:222:ASP:C	1:D:224:LEU:N	2.71	0.43
2:B:217:MET:O	2:B:221:LYS:HG3	2.19	0.43
1:A:10:ARG:HG3	5:A:491:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:CG2	1:A:251:LEU:HD11	2.49	0.42
2:B:250:ASN:O	2:B:252:GLU:N	2.52	0.42
1:A:218:GLN:NE2	5:A:607:HOH:O	2.51	0.42
2:B:14:ARG:NH1	2:B:14:ARG:HB2	2.34	0.42
2:C:92:SER:HB2	2:C:94:PRO:HD2	1.99	0.42
1:D:138:ARG:NH2	1:D:200:GLU:OE2	2.50	0.42
5:A:768:HOH:O	2:C:241:GLU:HG3	2.18	0.42
2:B:1:MET:HG3	2:B:2:GLN:H	1.82	0.42
1:D:290:ILE:HA	1:D:293:ARG:HD3	2.00	0.42
2:C:92:SER:O	2:C:93:LYS:C	2.57	0.42
1:D:220:VAL:HG11	1:D:291:ALA:O	2.19	0.42
1:D:131:ALA:HB1	1:D:135:ARG:HD2	2.01	0.42
2:B:218:MET:HA	2:B:221:LYS:CG	2.46	0.42
1:A:68:ALA:HA	1:A:124:VAL:HG22	2.02	0.42
1:D:292:TYR:CD2	1:D:292:TYR:N	2.87	0.42
5:C:288:HOH:O	1:D:149:SER:HB2	2.18	0.42
2:C:125:ASP:OD1	2:C:126:PRO:HD2	2.20	0.41
2:B:203:LYS:NZ	5:B:1101:HOH:O	2.52	0.41
2:B:165:ASN:O	2:B:165:ASN:CG	2.57	0.41
1:D:4:PHE:CE1	1:D:8:MET:SD	3.13	0.41
2:B:227:ILE:O	2:B:227:ILE:HG22	2.20	0.41
2:C:168:LEU:HB3	2:C:231:ILE:CD1	2.49	0.41
1:D:213:ILE:HD12	1:D:290:ILE:HD13	2.03	0.41
1:D:218:GLN:O	1:D:221:ASP:N	2.53	0.41
1:D:226:VAL:HG23	1:D:227:THR:N	2.35	0.41
2:C:5:TRP:CH2	2:C:257:LEU:HD22	2.56	0.41
2:B:236:LYS:O	2:B:240:LEU:HG	2.21	0.41
2:C:130:ASP:HA	5:C:1175:HOH:O	2.20	0.41
2:B:254:MET:O	2:B:257:LEU:HB2	2.20	0.41
1:D:215:LEU:O	1:D:218:GLN:HB2	2.21	0.41
2:C:271:HIS:ND1	2:C:271:HIS:C	2.73	0.41
1:D:220:VAL:CG2	1:D:261:ALA:HB1	2.51	0.41
1:D:220:VAL:O	1:D:223:ILE:N	2.54	0.41
2:B:47:LEU:HD13	2:B:257:LEU:HD13	2.03	0.41
2:C:125:ASP:CG	2:C:128:ARG:HG3	2.41	0.41
1:A:152:LEU:C	1:A:152:LEU:HD23	2.41	0.41
1:D:246:THR:N	1:D:250:LYS:HZ2	2.18	0.40
1:D:262:ASP:O	1:D:266:ARG:HG3	2.21	0.40
2:C:1:MET:HE2	2:C:5:TRP:HB2	2.02	0.40
1:A:149:SER:HB2	5:B:596:HOH:O	2.21	0.40
1:D:75:ILE:HG21	1:D:147:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:SER:C	1:A:164:GLY:N	2.75	0.40
1:D:226:VAL:CG2	1:D:227:THR:N	2.84	0.40
2:B:237:GLU:O	2:B:241:GLU:CB	2.70	0.40
1:A:248:TYR:HB2	1:A:249:PRO:HD3	2.02	0.40

All (2) 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)
5:D:1138:HOH:O	5:D:1229:HOH:O[1_455]	2.16	0.04
5:A:861:HOH:O	5:C:297:HOH:O[4_555]	2.19	0.01

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	275/295 (93%)	267 (97%)	5 (2%)	3 (1%)	17	6
1	D	273/295 (92%)	250 (92%)	16 (6%)	7 (3%)	7	1
2	B	257/274 (94%)	243 (95%)	9 (4%)	5 (2%)	10	2
2	C	269/274 (98%)	249 (93%)	13 (5%)	7 (3%)	7	1
All	All	1074/1138 (94%)	1009 (94%)	43 (4%)	22 (2%)	9	2

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	93	LYS
2	B	227	ILE
2	B	247	HIS
2	C	227	ILE
2	C	247	HIS

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Mol	Chain	Res	Type
1	D	247	THR
1	D	290	ILE
1	A	167	GLU
2	B	225	GLN
2	C	225	GLN
1	D	217	PHE
1	D	254	VAL
1	A	227	THR
2	B	2	GLN
2	C	226	LEU
2	C	163	ASP
2	C	165	ASN
1	D	166	ALA
1	A	163	GLU
1	D	223	ILE
1	D	252	ILE
2	C	93	LYS

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	222/234 (95%)	216 (97%)	6 (3%)	52	43
1	D	220/234 (94%)	213 (97%)	7 (3%)	46	35
2	B	201/214 (94%)	197 (98%)	4 (2%)	63	57
2	C	211/214 (99%)	207 (98%)	4 (2%)	65	59
All	All	854/896 (95%)	833 (98%)	21 (2%)	55	47

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	90	ASN
1	A	95	ARG
1	A	135	ARG

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Mol	Chain	Res	Type
1	A	221	ASP
1	A	228	LYS
2	B	2	GLN
2	B	54	LEU
2	B	211	GLN
2	B	246	PHE
2	C	59	ARG
2	C	92	SER
2	C	128	ARG
2	C	262	SER
1	D	9	LEU
1	D	44	LYS
1	D	86	PRO
1	D	139	VAL
1	D	263	ARG
1	D	270	GLU
1	D	279	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	177	HIS
1	A	276	HIS
2	B	250	ASN
2	C	34	HIS
2	C	165	ASN
2	C	225	GLN
2	C	230	ASN
2	C	250	ASN
2	C	267	HIS
1	D	178	HIS
1	D	211	ASN
1	D	218	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
4	EDO	C	2001	-	3,3,3	0.88	0	2,2,2	0.59	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
4	EDO	C	2001	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	279/295 (94%)	-0.04	14 (5%) 32 35	15, 23, 44, 78	0
1	D	277/295 (93%)	0.72	49 (17%) 2 2	16, 28, 90, 100	0
2	B	259/274 (94%)	0.51	35 (13%) 4 4	18, 28, 103, 117	0
2	C	271/274 (98%)	0.55	32 (11%) 6 6	16, 31, 72, 101	0
All	All	1086/1138 (95%)	0.43	130 (11%) 6 6	15, 28, 89, 117	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	VAL	11.3
1	D	165	MET	10.3
1	D	224	LEU	9.7
2	B	246	PHE	9.5
1	D	166	ALA	9.3
2	C	270	HIS	8.8
2	B	249	LYS	8.7
2	B	259	ALA	8.3
2	B	227	ILE	8.3
1	D	223	ILE	8.0
2	C	268	HIS	7.2
2	B	250	ASN	7.2
1	D	227	THR	7.0
2	C	93	LYS	7.0
2	C	267	HIS	6.9
1	A	166	ALA	6.9
1	D	292	TYR	6.9
1	D	168	VAL	6.8
2	B	1	MET	6.7
2	B	231	ILE	6.6
2	C	227	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
2	C	269	HIS	6.1
1	D	252	ILE	6.0
1	D	295	ASN	5.9
1	D	164	GLY	5.7
1	D	251	LEU	5.7
2	C	225	GLN	5.6
1	D	254	VAL	5.6
2	C	262	SER	5.6
1	D	246	THR	5.4
2	B	247	HIS	5.2
1	D	167	GLU	5.2
1	D	169	GLY	5.0
2	B	225	GLN	5.0
1	A	295	ASN	4.8
1	D	162	SER	4.8
2	C	127	ALA	4.8
2	C	271	HIS	4.7
2	B	245	GLY	4.6
1	A	164	GLY	4.5
1	D	255	GLU	4.5
2	B	93	LYS	4.5
2	C	163	ASP	4.4
1	D	250	LYS	4.4
1	D	220	VAL	4.3
1	D	249	PRO	4.3
2	B	222	ASN	4.3
2	B	2	GLN	4.1
2	C	222	ASN	4.1
2	C	94	PRO	4.0
1	D	221	ASP	3.9
1	D	170	LEU	3.9
2	C	164	GLY	3.9
1	D	217	PHE	3.8
1	A	165	MET	3.8
2	C	126	PRO	3.7
1	D	258	LYS	3.7
1	A	167	GLU	3.6
1	D	225	ASP	3.6
2	C	265	ALA	3.6
2	B	221	LYS	3.6
2	B	248	GLY	3.5
2	C	266	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	227	THR	3.3
1	A	228	LYS	3.2
2	B	229	GLU	3.2
2	B	238	LEU	3.2
2	C	224	HIS	3.2
2	B	226	LEU	3.1
2	B	253	LEU	3.1
1	D	262	ASP	3.1
2	C	91	VAL	3.1
2	B	243	LEU	3.1
2	B	164	GLY	3.1
2	C	223	SER	3.1
2	C	165	ASN	3.1
1	D	266	ARG	3.0
2	B	251	ALA	3.0
1	D	184	LEU	2.9
2	B	235	LEU	2.9
1	A	163	GLU	2.9
1	A	245	LYS	2.9
1	D	163	GLU	2.8
2	B	254	MET	2.8
2	C	259	ALA	2.7
2	B	240	LEU	2.7
1	D	222	ASP	2.7
2	B	257	LEU	2.7
2	C	261	PRO	2.7
1	D	256	LYS	2.6
2	C	92	SER	2.6
2	C	226	LEU	2.6
1	A	294	ASP	2.6
2	C	260	GLU	2.6
1	A	226	VAL	2.6
1	D	289	TYR	2.6
2	B	242	GLU	2.6
2	B	223	SER	2.6
1	D	173	LEU	2.6
2	B	230	ASN	2.6
2	C	249	LYS	2.6
1	D	290	ILE	2.5
2	B	241	GLU	2.5
1	D	147	ILE	2.5
1	D	215	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	91	VAL	2.4
1	D	294	ASP	2.4
2	B	215	ARG	2.4
2	C	229	GLU	2.4
2	C	128	ARG	2.3
1	D	259	GLU	2.3
1	D	286	LEU	2.3
1	D	257	SER	2.3
1	A	117	LEU	2.3
2	C	246	PHE	2.3
1	D	96	GLY	2.3
1	D	291	ALA	2.3
1	A	162	SER	2.2
2	B	94	PRO	2.2
1	D	185	LEU	2.2
1	D	247	THR	2.2
1	D	95	ARG	2.2
1	D	263	ARG	2.2
1	D	172	HIS	2.1
2	C	247	HIS	2.1
2	B	244	GLY	2.1
2	B	165	ASN	2.1
2	C	162	VAL	2.0
1	A	274	HIS	2.0
1	D	253	GLY	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 carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	C	2001	4/4	0.98	0.17	4.10	16,17,19,19	0
3	MG	D	3001	1/1	0.75	0.10	-	69,69,69,69	0
3	MG	A	3002	1/1	0.97	0.12	-	37,37,37,37	0
3	MG	A	3003	1/1	0.82	0.28	-	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.