



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:50 PM GMT

PDB ID : 1HJ6
Title : ISOCITRATE DEHYDROGENASE S113E MUTANT COMPLEXED WITH
ISOPROPYLMALATE, NADP+ AND MAGNESIUM (FLASH-COOLED)
Authors : Doyle, S.A.; Beernink, P.T.; Koshland Junior, D.E.
Deposited on : 2001-01-08
Resolution : 2.00 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

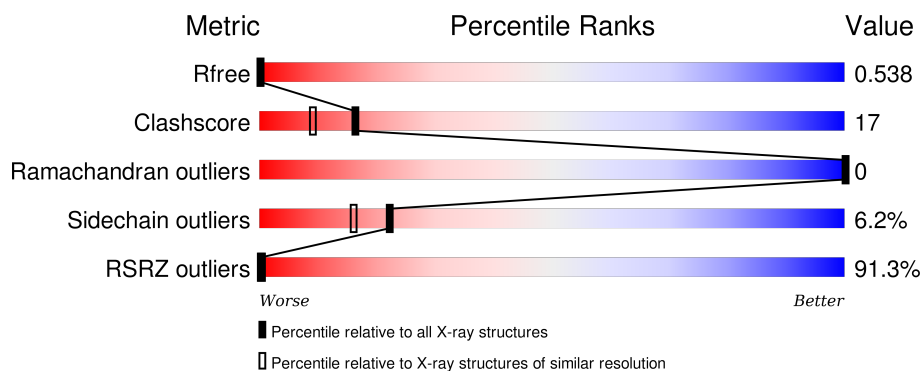
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	416	<div> <div>91%</div> <div>70%25%. </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	1417	-	X	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	1418	-	X	-	X
3	IPM	A	1419	-	-	-	X
5	MG	A	1421	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3504 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 ISOCITRATE DEHYDROGENASE.

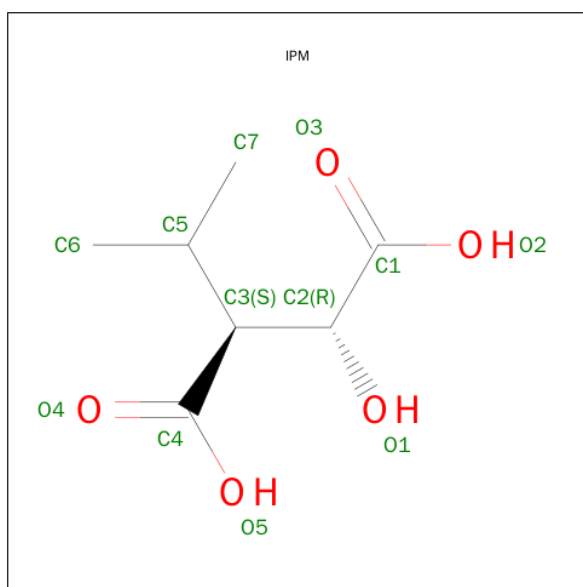
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3199	2037	538	606	18			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



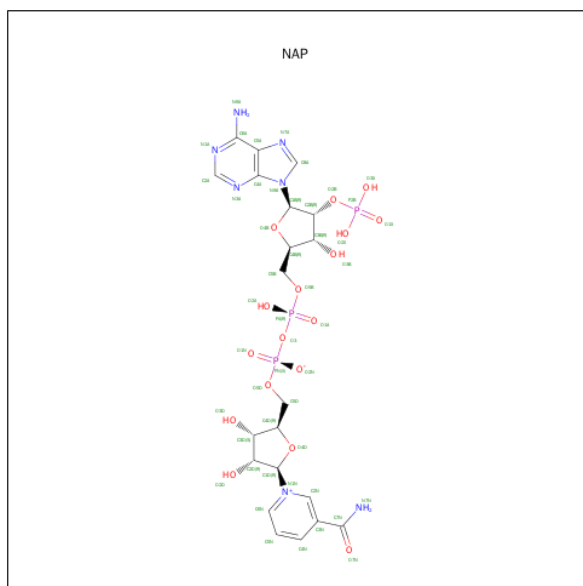
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 3-ISOPROPYLMALIC ACID (three-letter code: IPM) (formula: $C_7H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	7	5		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			48	21	7	17		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0

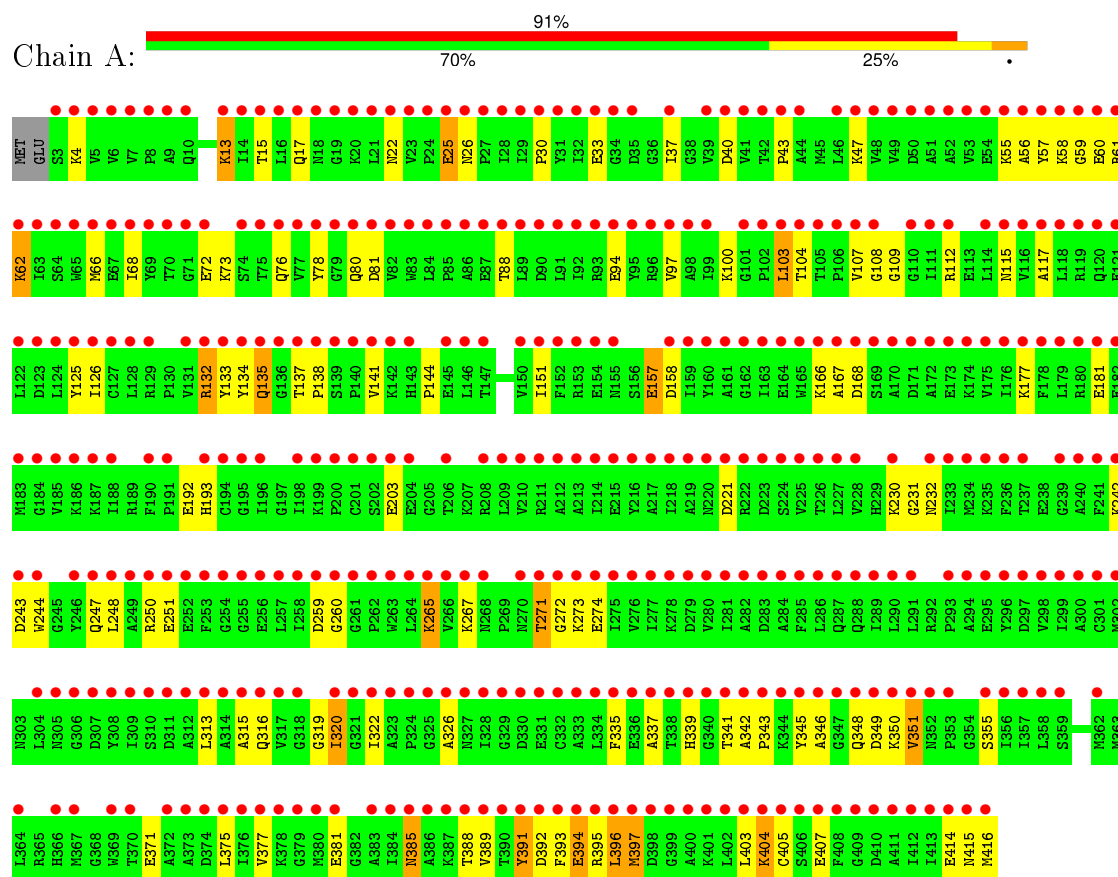
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	232	Total 232	O 232	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ISOCITRATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.30 Å 102.30 Å 150.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00 21.04 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.8 (6.00-2.00) 94.5 (21.04-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.95 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.206 , 0.246 0.530 , 0.538	Depositor DCC
R_{free} test set	2575 reflections (4.58%)	DCC
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 255.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 56169 reflections	Xtriage
F_o, F_c correlation	0.58	EDS
Total number of atoms	3504	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: GOL, NAP, MG, IPM

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	0.30	0/3260	0.56	0/4409

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3199	0	3223	109	50
2	A	12	0	8	0	0
3	A	12	0	10	0	0
4	A	48	0	25	0	0
5	A	1	0	0	0	0
6	A	232	0	0	38	1
All	All	3504	0	3266	109	51

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 17.

All (109) 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:415:ASN:N	6:A:2223:HOH:O	1.62	1.26
1:A:415:ASN:ND2	6:A:2223:HOH:O	1.63	1.24
1:A:59:GLY:CA	6:A:2033:HOH:O	1.86	1.21
1:A:416:MET:N	6:A:2224:HOH:O	1.78	1.16
1:A:109:GLY:CA	6:A:2077:HOH:O	1.93	1.15
1:A:80:GLN:CG	6:A:2056:HOH:O	2.00	1.07
1:A:232:ASN:N	6:A:2152:HOH:O	1.92	1.03
1:A:59:GLY:N	6:A:2033:HOH:O	1.93	0.96
1:A:80:GLN:HG3	6:A:2056:HOH:O	1.61	0.96
1:A:231:GLY:C	6:A:2152:HOH:O	2.01	0.95
1:A:109:GLY:O	6:A:2077:HOH:O	1.86	0.90
1:A:416:MET:O	6:A:2224:HOH:O	1.88	0.89
1:A:259:ASP:CG	1:A:260:GLY:H	1.77	0.86
1:A:415:ASN:CA	6:A:2223:HOH:O	2.10	0.84
1:A:80:GLN:OE1	6:A:2058:HOH:O	1.96	0.83
1:A:415:ASN:CG	6:A:2223:HOH:O	1.95	0.81
1:A:109:GLY:HA3	6:A:2077:HOH:O	1.69	0.79
1:A:415:ASN:CB	6:A:2223:HOH:O	2.22	0.79
1:A:349:ASP:OD1	1:A:405:CYS:HB3	1.85	0.76
1:A:404:LYS:HG2	1:A:407:GLU:H	1.52	0.73
1:A:80:GLN:NE2	6:A:2058:HOH:O	2.23	0.72
1:A:59:GLY:HA3	6:A:2033:HOH:O	1.70	0.72
1:A:80:GLN:HB2	6:A:2056:HOH:O	1.91	0.71
1:A:259:ASP:CG	1:A:260:GLY:N	2.47	0.68
1:A:138:PRO:HG3	1:A:393:PHE:O	1.93	0.68
1:A:80:GLN:O	1:A:81:ASP:HB2	1.92	0.68
1:A:231:GLY:CA	6:A:2152:HOH:O	2.36	0.67
1:A:80:GLN:CD	6:A:2058:HOH:O	2.33	0.67
1:A:414:GLU:C	6:A:2223:HOH:O	2.09	0.65
1:A:416:MET:CA	6:A:2224:HOH:O	2.37	0.65
1:A:76:GLN:HG2	6:A:2053:HOH:O	1.97	0.63
1:A:112:ARG:HD2	1:A:117:ALA:HB2	1.79	0.63
1:A:13:LYS:HE2	1:A:94:GLU:HG2	1.80	0.62
1:A:80:GLN:CD	6:A:2056:HOH:O	2.27	0.61
1:A:267:LYS:HD2	1:A:272:GLY:O	2.01	0.61
1:A:55:LYS:HG2	1:A:375:LEU:CD1	2.31	0.61
1:A:43:PRO:O	1:A:47:LYS:HG3	2.01	0.60
1:A:192:GLU:HB3	1:A:193:HIS:CD2	2.37	0.59
1:A:337:ALA:HB1	1:A:355:SER:HB3	1.85	0.59
1:A:138:PRO:HB3	1:A:397:MET:HG2	1.85	0.58
1:A:138:PRO:HG3	1:A:397:MET:HG3	1.86	0.58
1:A:377:VAL:O	1:A:381:GLU:HG3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:HG2	1:A:265:LYS:O	2.03	0.57
1:A:13:LYS:HE2	1:A:94:GLU:CG	2.35	0.57
1:A:404:LYS:HG2	1:A:407:GLU:HB2	1.88	0.55
1:A:404:LYS:CE	1:A:407:GLU:HG3	2.37	0.55
1:A:395:ARG:HD3	6:A:2218:HOH:O	2.07	0.54
1:A:151:ILE:HD11	1:A:313:LEU:HD12	1.88	0.54
1:A:80:GLN:CB	6:A:2056:HOH:O	2.35	0.53
1:A:55:LYS:HG2	1:A:375:LEU:HD11	1.89	0.53
1:A:177:LYS:O	1:A:181:GLU:HB2	2.09	0.53
1:A:341:THR:O	1:A:342:ALA:C	2.48	0.52
1:A:391:TYR:CG	1:A:392:ASP:N	2.78	0.52
1:A:313:LEU:O	1:A:316:GLN:HB2	2.10	0.52
1:A:388:THR:HB	1:A:403:LEU:HD11	1.92	0.52
1:A:404:LYS:HE2	1:A:407:GLU:HG3	1.92	0.52
1:A:132:ARG:HD2	1:A:134:TYR:CE1	2.46	0.51
1:A:230:LYS:HE3	1:A:232:ASN:OD1	2.11	0.51
1:A:393:PHE:O	1:A:397:MET:HG3	2.12	0.50
1:A:133:TYR:CD1	1:A:144:PRO:HB2	2.47	0.50
1:A:267:LYS:HD3	1:A:274:GLU:OE2	2.12	0.50
1:A:251:GLU:HG2	6:A:2162:HOH:O	2.11	0.49
1:A:345:TYR:O	1:A:348:GLN:HB2	2.12	0.49
1:A:158:ASP:HB2	6:A:2098:HOH:O	2.14	0.48
1:A:30:PRO:HA	1:A:66:MET:O	2.13	0.48
1:A:80:GLN:NE2	6:A:2056:HOH:O	2.45	0.48
1:A:73:LYS:HA	1:A:76:GLN:OE1	2.14	0.48
1:A:396:LEU:O	1:A:396:LEU:HD23	2.14	0.47
1:A:40:ASP:O	1:A:43:PRO:HD2	2.14	0.47
1:A:192:GLU:HB2	6:A:2132:HOH:O	2.14	0.47
1:A:177:LYS:HZ2	1:A:181:GLU:CD	2.18	0.47
1:A:26:ASN:HA	1:A:62:LYS:O	2.15	0.47
1:A:141:VAL:HG11	1:A:316:GLN:HG2	1.98	0.47
1:A:157:GLU:HB2	1:A:158:ASP:H	1.47	0.46
1:A:37:ILE:HB	1:A:351:VAL:HG21	1.96	0.46
1:A:166:LYS:NZ	6:A:2112:HOH:O	2.32	0.46
1:A:33:GLU:HG2	6:A:2015:HOH:O	2.16	0.46
1:A:343:PRO:HA	1:A:346:ALA:HB2	1.98	0.45
1:A:17:GLN:HE22	1:A:22:ASN:HD22	1.63	0.45
1:A:133:TYR:CE1	1:A:137:THR:HB	2.52	0.45
1:A:389:VAL:HG21	1:A:397:MET:HE2	1.99	0.45
1:A:30:PRO:HD2	1:A:97:VAL:O	2.17	0.44
1:A:273:LYS:HD2	6:A:2147:HOH:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:HZ3	1:A:100:LYS:HG3	1.71	0.43
1:A:231:GLY:HA3	6:A:2152:HOH:O	2.14	0.43
1:A:404:LYS:HE3	1:A:407:GLU:HG3	2.00	0.43
1:A:389:VAL:HG21	1:A:397:MET:CE	2.48	0.43
1:A:15:THR:OG1	1:A:22:ASN:HB3	2.18	0.43
1:A:247:GLN:NE2	6:A:2158:HOH:O	2.48	0.43
1:A:403:LEU:HD22	1:A:407:GLU:HB3	2.00	0.43
1:A:320:ILE:HD13	1:A:339:HIS:HA	2.01	0.42
1:A:17:GLN:NE2	1:A:22:ASN:HD22	2.17	0.42
1:A:326:ALA:HB2	1:A:335:PHE:CD2	2.54	0.42
1:A:221:ASP:CG	1:A:271:THR:HG21	2.38	0.42
1:A:394:GLU:O	1:A:397:MET:HB2	2.19	0.42
1:A:395:ARG:O	1:A:396:LEU:HB3	2.20	0.42
1:A:167:ALA:O	1:A:168:ASP:HB2	2.20	0.42
1:A:315:ALA:HA	1:A:319:GLY:HA2	2.02	0.42
1:A:68:ILE:HD12	1:A:88:THR:HG23	2.02	0.41
1:A:103:LEU:HB2	1:A:115:ASN:HD21	1.84	0.41
1:A:388:THR:HB	1:A:403:LEU:CD1	2.50	0.41
1:A:4:LYS:HG3	1:A:78:TYR:CE2	2.55	0.41
1:A:59:GLY:HA2	6:A:2033:HOH:O	1.81	0.41
1:A:135:GLN:CD	1:A:385:ASN:HD21	2.24	0.41
1:A:322:ILE:HG23	1:A:322:ILE:O	2.21	0.41
1:A:203:GLU:HG3	1:A:244:TRP:CD1	2.56	0.41
1:A:125:TYR:CD1	1:A:126:ILE:HG13	2.56	0.40
1:A:57:TYR:CD2	1:A:61:ARG:HD2	2.55	0.40
1:A:395:ARG:O	1:A:396:LEU:CB	2.69	0.40

All (51) 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:A:109:GLY:N	1:A:371:GLU:OE2[4_535]	0.62	1.58
1:A:250:ARG:NH2	1:A:414:GLU:C[5_354]	0.75	1.45
1:A:56:ALA:C	1:A:107:VAL:CB[3_344]	0.80	1.40
1:A:109:GLY:CA	1:A:371:GLU:OE2[4_535]	0.95	1.25
1:A:109:GLY:N	1:A:371:GLU:CD[4_535]	0.97	1.23
1:A:56:ALA:O	1:A:107:VAL:CB[3_344]	0.98	1.22
1:A:250:ARG:NH2	1:A:414:GLU:CA[5_354]	1.14	1.06
1:A:250:ARG:CZ	1:A:414:GLU:CA[5_354]	1.14	1.06
1:A:57:TYR:N	1:A:107:VAL:CG2[3_344]	1.18	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ALA:C	1:A:107:VAL:CG2[3_344]	1.28	0.92
1:A:56:ALA:CA	1:A:107:VAL:CG1[3_344]	1.32	0.88
1:A:56:ALA:C	1:A:107:VAL:CG1[3_344]	1.35	0.85
1:A:250:ARG:NE	1:A:414:GLU:CA[5_354]	1.42	0.78
1:A:250:ARG:NH2	1:A:414:GLU:O[5_354]	1.43	0.77
1:A:56:ALA:O	1:A:107:VAL:CG1[3_344]	1.44	0.76
1:A:56:ALA:O	1:A:107:VAL:CA[3_344]	1.50	0.70
1:A:60:GLU:OE1	1:A:104:THR:CG2[3_344]	1.53	0.67
1:A:250:ARG:NE	1:A:414:GLU:CG[5_354]	1.56	0.64
1:A:57:TYR:N	1:A:107:VAL:CB[3_344]	1.58	0.62
1:A:57:TYR:CA	1:A:107:VAL:CG2[3_344]	1.59	0.61
1:A:250:ARG:NE	1:A:414:GLU:CB[5_354]	1.60	0.60
1:A:56:ALA:O	1:A:107:VAL:CG2[3_344]	1.61	0.59
1:A:57:TYR:CE1	1:A:107:VAL:O[3_344]	1.61	0.59
1:A:250:ARG:CB	1:A:414:GLU:CG[5_354]	1.70	0.50
1:A:108:GLY:CA	1:A:371:GLU:CG[4_535]	1.72	0.48
1:A:250:ARG:CD	1:A:414:GLU:CG[5_354]	1.85	0.35
1:A:108:GLY:C	1:A:371:GLU:CD[4_535]	1.87	0.33
1:A:108:GLY:C	1:A:371:GLU:OE2[4_535]	1.87	0.33
1:A:25:GLU:OE1	1:A:72:GLU:OE1[3_344]	1.88	0.32
1:A:109:GLY:N	1:A:371:GLU:CG[4_535]	1.90	0.30
1:A:250:ARG:CB	1:A:414:GLU:CD[5_354]	1.91	0.29
1:A:250:ARG:NH2	1:A:415:ASN:N[5_354]	1.94	0.26
1:A:109:GLY:CA	1:A:371:GLU:CD[4_535]	2.00	0.20
1:A:60:GLU:OE2	1:A:104:THR:OG1[3_344]	2.02	0.18
1:A:109:GLY:C	1:A:371:GLU:OE2[4_535]	2.02	0.18
1:A:250:ARG:CZ	1:A:414:GLU:C[5_354]	2.04	0.16
1:A:57:TYR:CD1	1:A:107:VAL:N[3_344]	2.07	0.13
1:A:109:GLY:N	1:A:371:GLU:OE1[4_535]	2.07	0.13
1:A:55:LYS:NZ	1:A:243:ASP:OD2[5_344]	2.07	0.13
1:A:60:GLU:CD	1:A:104:THR:CG2[3_344]	2.09	0.11
1:A:108:GLY:C	1:A:371:GLU:CG[4_535]	2.11	0.09
1:A:250:ARG:CG	1:A:414:GLU:CG[5_354]	2.11	0.09
1:A:56:ALA:CA	1:A:107:VAL:CB[3_344]	2.11	0.09
1:A:60:GLU:CD	1:A:104:THR:OG1[3_344]	2.11	0.09
1:A:250:ARG:CZ	1:A:414:GLU:N[5_354]	2.12	0.08
6:A:2032:HOH:O	6:A:2152:HOH:O[5_344]	2.15	0.05
1:A:25:GLU:CD	1:A:72:GLU:OE1[3_344]	2.16	0.04
1:A:56:ALA:CB	1:A:107:VAL:CG1[3_344]	2.16	0.04
1:A:55:LYS:CE	1:A:243:ASP:OD1[5_344]	2.16	0.04
1:A:57:TYR:CD1	1:A:107:VAL:O[3_344]	2.17	0.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:NE	1:A:414:GLU:N[5_354]	2.17	0.03

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	412/416 (99%)	388 (94%)	24 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	336/338 (99%)	315 (94%)	21 (6%)	22	16

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

Mol	Chain	Res	Type
1	A	13	LYS
1	A	25	GLU
1	A	58	LYS
1	A	62	LYS
1	A	103	LEU
1	A	132	ARG
1	A	135	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	157	GLU
1	A	242	LYS
1	A	248	LEU
1	A	265	LYS
1	A	271	THR
1	A	320	ILE
1	A	350	LYS
1	A	351	VAL
1	A	385	ASN
1	A	391	TYR
1	A	394	GLU
1	A	396	LEU
1	A	397	MET
1	A	404	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	80	GLN
1	A	115	ASN
1	A	135	GLN
1	A	193	HIS
1	A	270	ASN
1	A	288	GLN
1	A	316	GLN
1	A	385	ASN

5.3.3 RNA [i](#)

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

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
2	GOL	A	1417	-	5,5,5	4.59	4 (80%)	5,5,5	5.72	3 (60%)
2	GOL	A	1418	-	5,5,5	4.59	4 (80%)	5,5,5	5.70	3 (60%)
3	IPM	A	1419	5	4,11,11	0.73	0	6,15,15	0.62	0
4	NAP	A	1420	-	42,52,52	1.50	8 (19%)	54,80,80	2.64	15 (27%)

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	GOL	A	1417	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1418	-	-	0/4/4/4	0/0/0/0
3	IPM	A	1419	5	-	0/8/16/16	0/0/0/0
4	NAP	A	1420	-	-	0/27/67/67	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1418	GOL	C3-C2	-8.11	1.21	1.52
2	A	1417	GOL	C3-C2	-8.07	1.21	1.52
4	A	1420	NAP	C3N-C7N	-4.14	1.44	1.50
2	A	1417	GOL	O2-C2	-2.81	1.35	1.43
2	A	1418	GOL	O2-C2	-2.72	1.35	1.43
4	A	1420	NAP	C8A-N7A	-2.21	1.30	1.34
4	A	1420	NAP	C5N-C4N	2.30	1.43	1.38
4	A	1420	NAP	C2N-C3N	2.34	1.42	1.39
4	A	1420	NAP	C4N-C3N	2.39	1.43	1.39
4	A	1420	NAP	C6N-N1N	2.89	1.43	1.35
4	A	1420	NAP	C4A-N3A	3.18	1.40	1.35
2	A	1418	GOL	O3-C3	3.33	1.56	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1417	GOL	O3-C3	3.43	1.57	1.42
4	A	1420	NAP	C2A-N3A	3.89	1.39	1.32
2	A	1417	GOL	O1-C1	4.49	1.61	1.42
2	A	1418	GOL	O1-C1	4.54	1.61	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1420	NAP	N3A-C2A-N1A	-9.22	121.83	128.89
4	A	1420	NAP	C3B-C2B-C1B	-3.86	95.26	102.73
4	A	1420	NAP	O4B-C1B-C2B	-2.41	102.25	106.60
4	A	1420	NAP	O4B-C4B-C3B	-2.30	100.52	105.15
4	A	1420	NAP	O7N-C7N-N7N	-2.27	119.40	122.59
4	A	1420	NAP	O5D-PN-O1N	-2.09	101.51	109.62
4	A	1420	NAP	O3B-C3B-C2B	2.03	117.02	111.16
4	A	1420	NAP	O2N-PN-O1N	2.14	124.13	112.53
4	A	1420	NAP	O3B-C3B-C4B	2.20	117.66	111.05
4	A	1420	NAP	C2A-N1A-C6A	2.28	122.84	118.77
4	A	1420	NAP	O5B-C5B-C4B	2.32	117.66	109.12
4	A	1420	NAP	C4D-O4D-C1D	2.65	112.63	109.72
4	A	1420	NAP	C3N-C7N-N7N	3.16	121.27	117.82
2	A	1417	GOL	O1-C1-C2	3.23	125.86	110.18
2	A	1418	GOL	O1-C1-C2	3.24	125.88	110.18
4	A	1420	NAP	O4B-C1B-N9A	6.54	121.79	108.10
2	A	1418	GOL	O2-C2-C3	6.57	138.79	108.65
2	A	1417	GOL	O2-C2-C3	6.60	138.94	108.65
2	A	1418	GOL	O3-C3-C2	10.42	160.71	110.18
2	A	1417	GOL	O3-C3-C2	10.43	160.79	110.18
4	A	1420	NAP	O4D-C1D-N1N	11.66	120.95	108.13

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	414/416 (99%)	4.76	378 (91%) 0 0	20, 31, 57, 90	0

All (378) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	GLY	23.8
1	A	77	VAL	16.9
1	A	385	ASN	15.8
1	A	4	LYS	14.9
1	A	398	ASP	13.1
1	A	405	CYS	13.1
1	A	255	GLY	12.8
1	A	294	ALA	12.7
1	A	400	ALA	12.7
1	A	58	LYS	12.1
1	A	271	THR	12.0
1	A	7	VAL	11.2
1	A	233	ILE	10.8
1	A	219	ALA	10.6
1	A	18	ASN	10.4
1	A	300	ALA	10.4
1	A	264	LEU	10.2
1	A	64	SER	10.2
1	A	272	GLY	9.9
1	A	415	ASN	9.4
1	A	78	TYR	9.4
1	A	76	GLN	9.4
1	A	47	LYS	9.3
1	A	401	LYS	9.1
1	A	388	THR	8.8
1	A	176	ILE	8.7
1	A	22	ASN	8.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	393	PHE	8.7
1	A	170	ALA	8.6
1	A	322	ILE	8.6
1	A	342	ALA	8.5
1	A	169	SER	8.4
1	A	182	GLU	8.4
1	A	63	ILE	8.4
1	A	17	GLN	8.3
1	A	356	ILE	8.3
1	A	190	PHE	8.3
1	A	184	GLY	8.2
1	A	139	SER	8.1
1	A	257	LEU	8.0
1	A	397	MET	8.0
1	A	80	GLN	7.9
1	A	364	LEU	7.9
1	A	399	GLY	7.8
1	A	254	GLY	7.8
1	A	384	ILE	7.5
1	A	168	ASP	7.4
1	A	92	ILE	7.4
1	A	133	TYR	7.4
1	A	16	LEU	7.3
1	A	186	LYS	7.3
1	A	3	SER	7.3
1	A	389	VAL	7.2
1	A	194	CYS	7.2
1	A	146	LEU	7.2
1	A	8	PRO	7.1
1	A	27	PRO	7.1
1	A	251	GLU	7.0
1	A	51	ALA	7.0
1	A	344	LYS	6.9
1	A	216	TYR	6.9
1	A	5	VAL	6.9
1	A	54	GLU	6.8
1	A	175	VAL	6.8
1	A	386	ALA	6.8
1	A	188	ILE	6.7
1	A	141	VAL	6.7
1	A	66	MET	6.6
1	A	295	GLU	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	228	VAL	6.6
1	A	50	ASP	6.6
1	A	250	ARG	6.5
1	A	350	LYS	6.5
1	A	345	TYR	6.4
1	A	396	LEU	6.4
1	A	68	ILE	6.4
1	A	14	ILE	6.3
1	A	328	ILE	6.3
1	A	131	VAL	6.3
1	A	124	LEU	6.3
1	A	137	THR	6.3
1	A	259	ASP	6.3
1	A	43	PRO	6.2
1	A	106	PRO	6.2
1	A	256	GLU	6.2
1	A	387	LYS	6.1
1	A	56	ALA	6.1
1	A	19	GLY	6.0
1	A	110	GLY	6.0
1	A	260	GLY	6.0
1	A	99	ILE	6.0
1	A	379	GLY	6.0
1	A	253	PHE	6.0
1	A	402	LEU	5.9
1	A	116	VAL	5.9
1	A	20	LYS	5.9
1	A	150	VAL	5.9
1	A	86	ALA	5.9
1	A	136	GLY	5.9
1	A	346	ALA	5.9
1	A	57	TYR	5.9
1	A	275	ILE	5.8
1	A	39	VAL	5.8
1	A	353	PRO	5.8
1	A	332	CYS	5.8
1	A	10	GLN	5.8
1	A	183	MET	5.8
1	A	23	VAL	5.8
1	A	414	GLU	5.8
1	A	243	ASP	5.7
1	A	97	VAL	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	134	TYR	5.7
1	A	394	GLU	5.7
1	A	404	LYS	5.7
1	A	222	ARG	5.6
1	A	377	VAL	5.6
1	A	142	LYS	5.6
1	A	357	ILE	5.6
1	A	21	LEU	5.5
1	A	191	PRO	5.5
1	A	284	ALA	5.5
1	A	321	GLY	5.5
1	A	281	ILE	5.5
1	A	67	GLU	5.4
1	A	185	VAL	5.4
1	A	81	ASP	5.4
1	A	330	ASP	5.4
1	A	338	THR	5.4
1	A	114	LEU	5.3
1	A	91	LEU	5.3
1	A	31	TYR	5.3
1	A	369	TRP	5.3
1	A	98	ALA	5.3
1	A	268	ASN	5.3
1	A	193	HIS	5.2
1	A	198	ILE	5.2
1	A	241	PHE	5.2
1	A	95	TYR	5.2
1	A	143	HIS	5.2
1	A	107	VAL	5.2
1	A	132	ARG	5.2
1	A	102	PRO	5.2
1	A	248	LEU	5.2
1	A	301	CYS	5.2
1	A	263	TRP	5.1
1	A	89	LEU	5.1
1	A	174	LYS	5.1
1	A	111	ILE	5.0
1	A	196	ILE	5.0
1	A	6	VAL	5.0
1	A	324	PRO	5.0
1	A	351	VAL	5.0
1	A	302	MET	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	362	MET	5.0
1	A	337	ALA	5.0
1	A	410	ASP	5.0
1	A	210	VAL	5.0
1	A	217	ALA	5.0
1	A	128	LEU	4.9
1	A	33	GLU	4.9
1	A	391	TYR	4.9
1	A	244	TRP	4.9
1	A	266	VAL	4.9
1	A	258	ILE	4.9
1	A	171	ASP	4.8
1	A	212	ALA	4.8
1	A	249	ALA	4.8
1	A	316	GLN	4.8
1	A	296	TYR	4.8
1	A	26	ASN	4.8
1	A	42	THR	4.8
1	A	293	PRO	4.8
1	A	83	TRP	4.7
1	A	317	VAL	4.7
1	A	34	GLY	4.7
1	A	159	ILE	4.7
1	A	40	ASP	4.7
1	A	311	ASP	4.7
1	A	29	ILE	4.7
1	A	227	LEU	4.7
1	A	112	ARG	4.7
1	A	117	ALA	4.6
1	A	290	LEU	4.6
1	A	392	ASP	4.6
1	A	178	PHE	4.6
1	A	79	GLY	4.6
1	A	28	ILE	4.6
1	A	147	THR	4.5
1	A	69	TYR	4.5
1	A	390	THR	4.5
1	A	366	HIS	4.5
1	A	62	LYS	4.5
1	A	372	ALA	4.5
1	A	320	ILE	4.5
1	A	105	THR	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	125	TYR	4.5
1	A	88	THR	4.5
1	A	370	THR	4.4
1	A	59	GLY	4.4
1	A	252	GLU	4.4
1	A	333	ALA	4.4
1	A	122	LEU	4.4
1	A	225	VAL	4.3
1	A	265	LYS	4.3
1	A	82	VAL	4.3
1	A	74	SER	4.3
1	A	163	ILE	4.3
1	A	15	THR	4.3
1	A	177	LYS	4.3
1	A	49	VAL	4.3
1	A	138	PRO	4.2
1	A	84	LEU	4.2
1	A	209	LEU	4.2
1	A	223	ASP	4.2
1	A	286	LEU	4.2
1	A	103	LEU	4.2
1	A	407	GLU	4.1
1	A	119	ARG	4.1
1	A	221	ASP	4.1
1	A	61	ARG	4.1
1	A	277	ILE	4.1
1	A	395	ARG	4.1
1	A	276	VAL	4.1
1	A	413	ILE	4.1
1	A	127	CYS	4.0
1	A	204	GLU	4.0
1	A	30	PRO	4.0
1	A	289	ILE	4.0
1	A	55	LYS	4.0
1	A	297	ASP	4.0
1	A	412	ILE	4.0
1	A	323	ALA	3.9
1	A	373	ALA	3.9
1	A	288	GLN	3.9
1	A	41	VAL	3.9
1	A	93	ARG	3.9
1	A	242	LYS	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	104	THR	3.9
1	A	172	ALA	3.9
1	A	215	GLU	3.9
1	A	262	PRO	3.9
1	A	179	LEU	3.9
1	A	235	LYS	3.8
1	A	246	TYR	3.8
1	A	403	LEU	3.8
1	A	180	ARG	3.8
1	A	200	PRO	3.8
1	A	52	ALA	3.8
1	A	96	ARG	3.8
1	A	375	LEU	3.8
1	A	347	GLY	3.8
1	A	408	PHE	3.8
1	A	161	ALA	3.7
1	A	48	VAL	3.7
1	A	201	CYS	3.7
1	A	151	ILE	3.7
1	A	335	PHE	3.7
1	A	329	GLY	3.7
1	A	299	ILE	3.7
1	A	9	ALA	3.7
1	A	126	ILE	3.7
1	A	181	GLU	3.6
1	A	298	VAL	3.6
1	A	65	TRP	3.6
1	A	358	LEU	3.6
1	A	376	ILE	3.6
1	A	339	HIS	3.6
1	A	53	VAL	3.6
1	A	46	LEU	3.6
1	A	224	SER	3.5
1	A	158	ASP	3.5
1	A	152	PHE	3.5
1	A	32	ILE	3.5
1	A	90	ASP	3.5
1	A	153	ARG	3.5
1	A	287	GLN	3.5
1	A	310	SER	3.4
1	A	318	GLY	3.4
1	A	165	TRP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	304	LEU	3.4
1	A	37	ILE	3.4
1	A	214	ILE	3.4
1	A	25	GLU	3.4
1	A	341	THR	3.4
1	A	352	ASN	3.4
1	A	24	PRO	3.4
1	A	145	GLU	3.3
1	A	234	MET	3.3
1	A	232	ASN	3.3
1	A	173	GLU	3.3
1	A	378	LYS	3.3
1	A	247	GLN	3.3
1	A	236	PHE	3.2
1	A	206	THR	3.2
1	A	409	GLY	3.2
1	A	406	SER	3.2
1	A	313	LEU	3.2
1	A	118	LEU	3.2
1	A	283	ASP	3.2
1	A	60	GLU	3.2
1	A	334	LEU	3.2
1	A	380	MET	3.1
1	A	218	ILE	3.1
1	A	94	GLU	3.1
1	A	274	GLU	3.1
1	A	220	ASN	3.1
1	A	202	SER	3.1
1	A	72	GLU	3.1
1	A	160	TYR	3.1
1	A	279	ASP	3.1
1	A	85	PRO	3.1
1	A	383	ALA	3.0
1	A	71	GLY	3.0
1	A	164	GLU	3.0
1	A	355	SER	3.0
1	A	239	GLY	3.0
1	A	213	ALA	3.0
1	A	87	GLU	2.9
1	A	349	ASP	2.9
1	A	70	THR	2.9
1	A	308	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	240	ALA	2.9
1	A	155	ASN	2.9
1	A	343	PRO	2.9
1	A	327	ASN	2.9
1	A	140	PRO	2.9
1	A	123	ASP	2.9
1	A	367	MET	2.8
1	A	166	LYS	2.8
1	A	270	ASN	2.8
1	A	280	VAL	2.8
1	A	416	MET	2.8
1	A	309	ILE	2.8
1	A	211	ARG	2.7
1	A	331	GLU	2.7
1	A	208	ARG	2.7
1	A	374	ASP	2.6
1	A	305	ASN	2.6
1	A	226	THR	2.6
1	A	195	GLY	2.6
1	A	325	GLY	2.6
1	A	13	LYS	2.6
1	A	359	SER	2.5
1	A	162	GLY	2.5
1	A	326	ALA	2.5
1	A	336	GLU	2.5
1	A	115	ASN	2.5
1	A	199	LYS	2.5
1	A	314	ALA	2.5
1	A	411	ALA	2.5
1	A	267	LYS	2.5
1	A	340	GLY	2.5
1	A	381	GLU	2.4
1	A	312	ALA	2.4
1	A	285	PHE	2.4
1	A	306	GLY	2.4
1	A	135	GLN	2.4
1	A	237	THR	2.4
1	A	278	LYS	2.4
1	A	35	ASP	2.4
1	A	120	GLN	2.4
1	A	101	GLY	2.4
1	A	282	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	291	LEU	2.3
1	A	129	ARG	2.3
1	A	315	ALA	2.3
1	A	121	GLU	2.2
1	A	187	LYS	2.2
1	A	273	LYS	2.2
1	A	261	GLY	2.2
1	A	154	GLU	2.2
1	A	307	ASP	2.2
1	A	230	LYS	2.1
1	A	203	GLU	2.1
1	A	348	GLN	2.1
1	A	167	ALA	2.1
1	A	44	ALA	2.1
1	A	75	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [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. 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(Å ²)	Q<0.9
5	MG	A	1421	1/1	0.08	0.53	3.32	26,26,26,26	0
2	GOL	A	1417	6/6	0.01	0.56	3.29	67,83,85,87	0
3	IPM	A	1419	12/12	0.44	0.49	1.54	25,29,34,37	0
2	GOL	A	1418	6/6	0.00	0.41	0.87	64,71,73,75	0
4	NAP	A	1420	48/48	0.60	0.32	-0.40	28,47,53,56	0

6.5 Other polymers

There are no such residues in this entry.