Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2023 – 10:03 PM EDT

PDB ID	:	1HU9
Title	:	LIPOXYGENASE-3 (SOYBEAN) COMPLEX WITH 4-HYDROPEROXY-2 -METHOXY-PHENOL
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Deposited on	:	2001-01-04
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

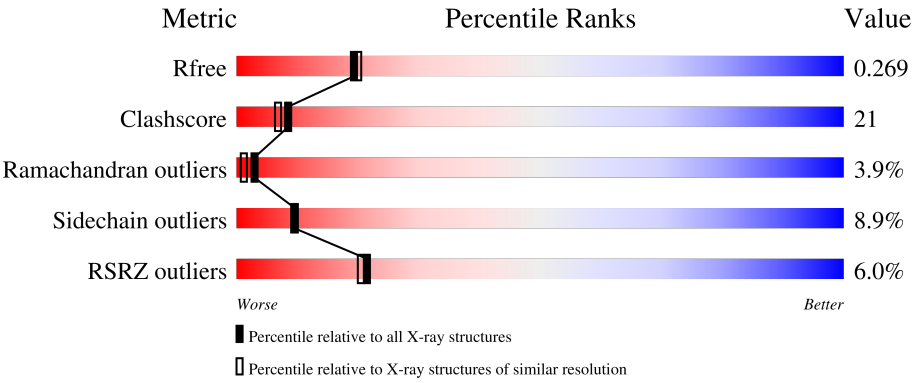
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	857	6% 62% 30% 7%

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
3	4HM	A	861	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7211 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 LIPOXYGENASE-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	849	Total	C	N	O	S	0	0	0
			6778	4329	1163	1268	18			

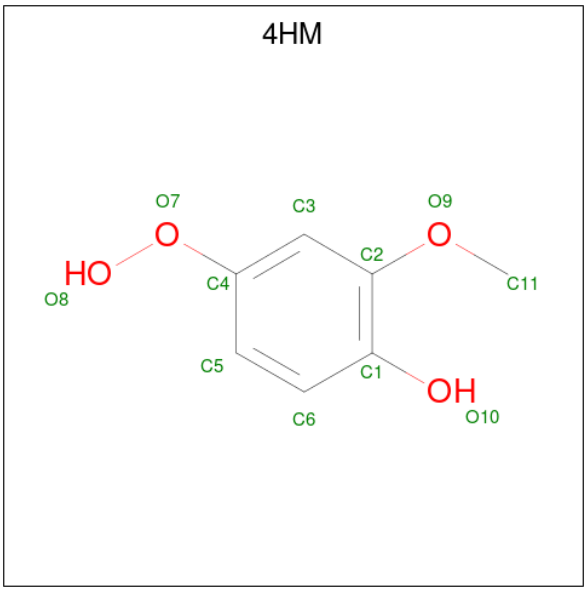
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASP	HIS	SEE REMARK 999	UNP P09186
A	57	SER	PRO	SEE REMARK 999	UNP P09186
A	112	PRO	LEU	SEE REMARK 999	UNP P09186
A	201	ILE	VAL	SEE REMARK 999	UNP P09186
A	382	ASP	GLU	SEE REMARK 999	UNP P09186
A	428	ASP	GLY	SEE REMARK 999	UNP P09186
A	630	THR	ALA	SEE REMARK 999	UNP P09186

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 4-HYDROPEROXY-2-METHOXY-PHENOL (three-letter code: 4HM) (formula: $C_7H_8O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 7 4	0	0

- Molecule 4 is water.

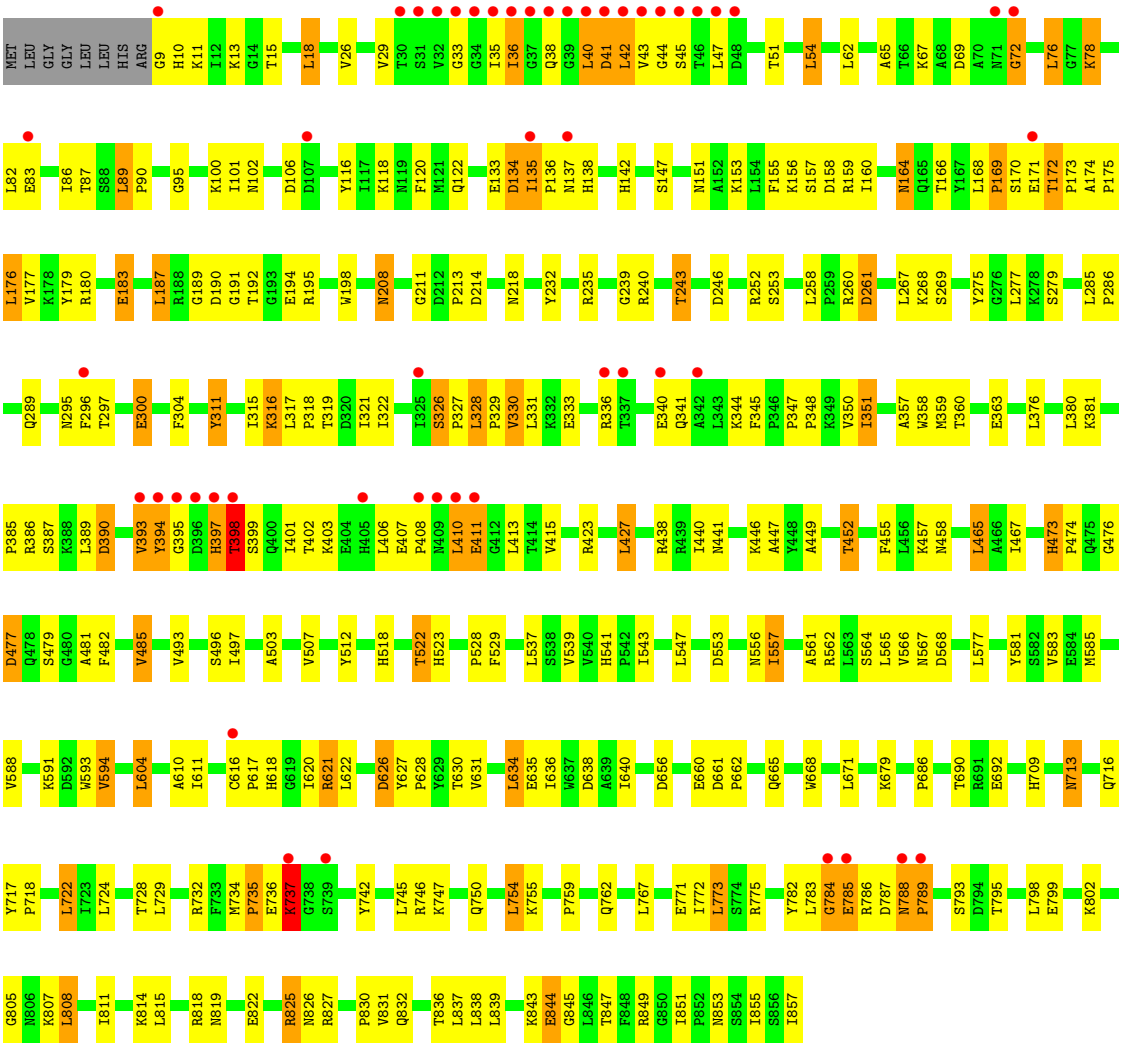
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	421	Total O 421 421	0	0

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: LIPOXYGENASE-3

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.79Å 137.32Å 61.87Å 90.00° 95.55° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 39.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	83.2 (40.00-2.20) 83.5 (39.62-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.185 , 0.271 0.182 , 0.269	Depositor DCC
R_{free} test set	4547 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 79.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7211	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 4HM

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	0.40	0/6950	0.71	3/9439 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	LEU	CA-CB-CG	6.91	131.20	115.30
1	A	729	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	449	ALA	N-CA-C	-5.02	97.44	111.00

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	6778	0	6701	280	0
2	A	1	0	0	0	0
3	A	11	0	6	4	0
4	A	421	0	0	22	0
All	All	7211	0	6707	280	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (280) 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:836:THR:HG22	1:A:849:ARG:HB3	1.35	1.08
1:A:393:VAL:HB	1:A:479:SER:HA	1.37	1.01
1:A:734:MET:HE3	1:A:735:PRO:HD2	1.42	1.01
1:A:135:ILE:HB	1:A:136:PRO:HD3	1.42	1.00
1:A:788:ASN:HB2	1:A:789:PRO:HD3	1.45	0.99
1:A:441:ASN:HD21	1:A:447:ALA:H	1.01	0.91
1:A:348:PRO:HD2	1:A:351:ILE:HD11	1.52	0.91
1:A:836:THR:HG23	1:A:839:LEU:HD22	1.52	0.90
1:A:289:GLN:HB2	4:A:1286:HOH:O	1.72	0.89
1:A:541:HIS:HD2	1:A:543:ILE:H	1.22	0.87
1:A:690:THR:HG22	1:A:692:GLU:H	1.41	0.86
1:A:847:THR:HG22	1:A:849:ARG:HG2	1.60	0.84
1:A:561:ALA:HA	1:A:565:LEU:HB2	1.58	0.84
1:A:522:THR:HG21	1:A:709:HIS:HD2	1.43	0.84
1:A:387:SER:HB3	1:A:395:GLY:HA2	1.57	0.83
1:A:192:THR:HG21	4:A:1272:HOH:O	1.76	0.83
1:A:318:PRO:HG2	1:A:321:ILE:HG12	1.60	0.82
1:A:604:LEU:HD21	1:A:630:THR:HG23	1.58	0.82
1:A:285:LEU:HB3	1:A:286:PRO:HD3	1.62	0.81
1:A:357:ALA:O	1:A:360:THR:HG22	1.80	0.81
1:A:326:SER:H	1:A:327:PRO:HD2	1.45	0.80
1:A:441:ASN:ND2	1:A:447:ALA:H	1.80	0.79
1:A:447:ALA:HB2	1:A:577:LEU:HD11	1.64	0.79
1:A:819:ASN:ND2	1:A:827:ARG:HE	1.80	0.79
1:A:522:THR:HG21	1:A:709:HIS:CD2	2.19	0.77
1:A:522:THR:HG22	1:A:523:HIS:N	2.00	0.77
1:A:496:SER:HB3	1:A:745:LEU:HD22	1.68	0.75
1:A:86:ILE:HG21	1:A:89:LEU:HD13	1.68	0.74
1:A:825:ARG:HE	1:A:825:ARG:HA	1.53	0.74
1:A:194:GLU:HA	1:A:239:GLY:HA3	1.70	0.74
1:A:304:PHE:H	1:A:750:GLN:NE2	1.86	0.74
1:A:616:CYS:SG	1:A:617:PRO:HD2	2.27	0.74
1:A:386:ARG:HB3	1:A:398:THR:HG22	1.68	0.74
1:A:213:PRO:HB2	1:A:243:THR:HG21	1.68	0.73
1:A:171:GLU:HG2	1:A:180:ARG:HD3	1.70	0.72
1:A:807:LYS:O	1:A:811:ILE:HG12	1.89	0.72
1:A:819:ASN:HD22	1:A:827:ARG:HE	1.35	0.72
1:A:171:GLU:HB2	1:A:177:VAL:HG22	1.71	0.72
1:A:423:ARG:HH22	1:A:458:ASN:ND2	1.89	0.71
1:A:799:GLU:HG2	4:A:1153:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:HD23	1:A:76:LEU:H	1.57	0.70
1:A:151:ASN:OD1	1:A:153:LYS:HG2	1.92	0.70
1:A:473:HIS:HB3	1:A:477:ASP:HA	1.73	0.70
1:A:240:ARG:HD3	1:A:253:SER:HB2	1.74	0.69
1:A:737:LYS:HA	1:A:742:TYR:CD2	2.26	0.69
1:A:360:THR:HG21	1:A:830:PRO:HG3	1.75	0.69
1:A:389:LEU:HD13	1:A:394:TYR:OH	1.93	0.68
1:A:36:ILE:HB	1:A:268:LYS:HG3	1.76	0.68
1:A:759:PRO:HG2	1:A:762:GLN:HE21	1.57	0.68
1:A:775:ARG:HG3	1:A:845:GLY:HA2	1.77	0.67
1:A:529:PHE:CD1	1:A:671:LEU:HD11	2.30	0.66
1:A:168:LEU:HD22	1:A:169:PRO:HD2	1.77	0.66
1:A:784:GLY:HA2	1:A:808:LEU:HD23	1.78	0.66
1:A:541:HIS:CD2	1:A:543:ILE:H	2.10	0.66
1:A:783:LEU:O	1:A:785:GLU:N	2.29	0.66
1:A:785:GLU:HB3	1:A:805:GLY:CA	2.25	0.65
1:A:135:ILE:HB	1:A:136:PRO:CD	2.22	0.65
1:A:795:THR:HG22	4:A:1068:HOH:O	1.97	0.65
1:A:397:HIS:O	1:A:398:THR:HG23	1.97	0.65
1:A:767:LEU:O	1:A:771:GLU:HB2	1.97	0.65
1:A:9:GLY:HA3	1:A:106:ASP:HA	1.78	0.64
1:A:142:HIS:HB2	4:A:909:HOH:O	1.96	0.64
1:A:380:LEU:HD11	1:A:385:PRO:HG3	1.78	0.64
1:A:381:LYS:HA	1:A:381:LYS:HE2	1.80	0.63
1:A:208:ASN:ND2	1:A:235:ARG:HH21	1.97	0.63
1:A:171:GLU:CG	1:A:180:ARG:HD3	2.30	0.62
1:A:319:THR:OG1	1:A:340:GLU:HG3	2.00	0.62
1:A:474:PRO:HB3	1:A:482:PHE:HB2	1.81	0.62
1:A:503:ALA:O	1:A:507:VAL:HG23	2.00	0.61
1:A:171:GLU:HA	1:A:180:ARG:HH11	1.64	0.61
1:A:183:GLU:O	1:A:187:LEU:HD22	2.01	0.60
1:A:211:GLY:HA2	1:A:568:ASP:HB2	1.83	0.60
1:A:661:ASP:O	1:A:665:GLN:HG2	2.02	0.60
1:A:173:PRO:HB2	1:A:176:LEU:HB2	1.84	0.60
1:A:160:ILE:CG2	1:A:183:GLU:HG3	2.31	0.60
1:A:566:VAL:HG22	1:A:583:VAL:HG22	1.83	0.59
1:A:243:THR:HG22	1:A:246:ASP:H	1.66	0.59
1:A:10:HIS:CG	1:A:11:LYS:H	2.20	0.59
1:A:566:VAL:HG22	1:A:583:VAL:CG2	2.33	0.59
1:A:692:GLU:HB2	4:A:1211:HOH:O	2.01	0.59
1:A:403:LYS:HE3	1:A:415:VAL:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:THR:HG22	1:A:692:GLU:N	2.16	0.59
1:A:762:GLN:H	1:A:762:GLN:NE2	2.01	0.59
1:A:836:THR:HG22	1:A:849:ARG:CB	2.24	0.58
1:A:348:PRO:HB2	1:A:350:VAL:HG12	1.85	0.58
1:A:493:VAL:HG21	1:A:746:ARG:HE	1.68	0.58
1:A:722:LEU:HD22	1:A:724:LEU:HB2	1.86	0.58
1:A:507:VAL:HG12	1:A:577:LEU:HD22	1.84	0.58
1:A:825:ARG:HA	1:A:825:ARG:NE	2.19	0.58
1:A:626:ASP:HB3	4:A:908:HOH:O	2.04	0.58
1:A:759:PRO:HG2	1:A:762:GLN:NE2	2.18	0.58
1:A:208:ASN:HD22	1:A:208:ASN:H	1.51	0.57
1:A:351:ILE:HD13	1:A:351:ILE:H	1.69	0.57
1:A:169:PRO:HG3	1:A:661:ASP:CG	2.24	0.57
1:A:168:LEU:HB3	1:A:169:PRO:HD2	1.86	0.57
1:A:618:HIS:HD2	1:A:638:ASP:OD2	1.88	0.57
1:A:836:THR:CG2	1:A:849:ARG:HB3	2.23	0.57
1:A:455:PHE:HB2	1:A:465:LEU:HD22	1.88	0.56
1:A:785:GLU:OE1	1:A:802:LYS:HA	2.06	0.56
1:A:168:LEU:CB	1:A:169:PRO:HD2	2.35	0.56
1:A:316:LYS:HD3	1:A:341:GLN:O	2.05	0.56
1:A:36:ILE:HB	1:A:268:LYS:CG	2.35	0.56
1:A:43:VAL:HB	1:A:87:THR:O	2.05	0.55
1:A:171:GLU:HA	1:A:180:ARG:NH1	2.21	0.55
1:A:348:PRO:HD2	1:A:351:ILE:CD1	2.31	0.55
1:A:671:LEU:HG	4:A:970:HOH:O	2.06	0.55
1:A:157:SER:O	1:A:158:ASP:HB2	2.07	0.55
1:A:399:SER:OG	1:A:401:ILE:HG12	2.05	0.55
1:A:616:CYS:SG	1:A:620:ILE:O	2.64	0.55
1:A:529:PHE:CE1	1:A:671:LEU:HD11	2.42	0.55
1:A:42:LEU:HD22	1:A:95:GLY:HA2	1.88	0.55
1:A:360:THR:HG23	1:A:363:GLU:H	1.70	0.55
1:A:713:ASN:ND2	1:A:716:GLN:HE21	2.05	0.55
1:A:785:GLU:HB3	1:A:805:GLY:HA3	1.88	0.54
1:A:656:ASP:O	1:A:660:GLU:HG3	2.07	0.54
1:A:394:TYR:HA	1:A:397:HIS:HB3	1.88	0.54
1:A:522:THR:HG22	1:A:523:HIS:H	1.72	0.54
1:A:260:ARG:O	1:A:261:ASP:HB2	2.08	0.54
1:A:438:ARG:HG2	4:A:960:HOH:O	2.06	0.54
1:A:51:THR:HA	1:A:54:LEU:HD22	1.90	0.54
1:A:541:HIS:HD2	1:A:543:ILE:N	2.01	0.53
1:A:581:TYR:HB2	1:A:585:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASP:CG	1:A:135:ILE:H	2.12	0.53
1:A:328:LEU:HD13	1:A:331:LEU:HB2	1.90	0.53
1:A:522:THR:CG2	1:A:523:HIS:N	2.71	0.53
1:A:476:GLY:O	1:A:477:ASP:HB2	2.09	0.53
1:A:668:TRP:HZ2	1:A:686:PRO:HD2	1.73	0.53
1:A:518:HIS:O	1:A:522:THR:HB	2.08	0.52
1:A:26:VAL:HG12	4:A:1285:HOH:O	2.09	0.52
1:A:843:LYS:HD3	4:A:1276:HOH:O	2.08	0.52
1:A:322:ILE:HG13	1:A:341:GLN:HA	1.90	0.52
1:A:782:TYR:O	1:A:786:ARG:HB2	2.09	0.52
1:A:171:GLU:CB	1:A:180:ARG:HD3	2.39	0.52
1:A:240:ARG:HD3	1:A:253:SER:CB	2.39	0.52
1:A:45:SER:OG	1:A:87:THR:HG23	2.10	0.52
1:A:340:GLU:HG2	1:A:341:GLN:HG3	1.91	0.51
1:A:10:HIS:HB3	1:A:135:ILE:HD13	1.91	0.51
1:A:844:GLU:HG2	1:A:845:GLY:N	2.24	0.51
1:A:819:ASN:HD21	1:A:827:ARG:HH21	1.59	0.51
1:A:588:VAL:O	1:A:591:LYS:HB2	2.10	0.51
1:A:120:PHE:HZ	4:A:1273:HOH:O	1.93	0.51
1:A:452:THR:HB	1:A:467:ILE:HG12	1.92	0.50
1:A:773:LEU:HD21	3:A:861:4HM:H5	1.93	0.50
1:A:557:ILE:HG13	1:A:857:ILE:HA	1.92	0.50
1:A:208:ASN:HD21	1:A:235:ARG:NH2	2.09	0.50
1:A:713:ASN:ND2	1:A:716:GLN:NE2	2.58	0.50
1:A:10:HIS:ND1	1:A:135:ILE:HG12	2.27	0.50
1:A:581:TYR:HB2	1:A:585:MET:HE3	1.93	0.50
1:A:116:TYR:HH	1:A:179:TYR:HE1	1.57	0.49
1:A:788:ASN:HB2	1:A:789:PRO:CD	2.31	0.49
1:A:208:ASN:ND2	1:A:235:ARG:NH2	2.59	0.49
1:A:11:LYS:HG2	1:A:102:ASN:HB3	1.93	0.49
1:A:410:LEU:CD1	1:A:411:GLU:H	2.25	0.49
1:A:626:ASP:HB2	1:A:826:ASN:ND2	2.28	0.49
1:A:825:ARG:HB3	4:A:912:HOH:O	2.11	0.49
1:A:279:SER:HB2	1:A:331:LEU:HD21	1.94	0.49
1:A:732:ARG:HH11	1:A:755:LYS:HB2	1.77	0.49
1:A:258:LEU:HD13	1:A:556:ASN:HA	1.94	0.49
1:A:750:GLN:O	1:A:754:LEU:HD22	2.12	0.49
1:A:42:LEU:HB2	1:A:95:GLY:H	1.77	0.49
1:A:192:THR:O	1:A:195:ARG:NH2	2.46	0.49
1:A:410:LEU:HG	1:A:457:LYS:HG2	1.95	0.49
1:A:528:PRO:HB2	4:A:970:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:VAL:HG11	1:A:577:LEU:HD13	1.95	0.48
1:A:522:THR:HG23	1:A:855:ILE:CD1	2.43	0.48
1:A:36:ILE:HG13	1:A:267:LEU:HB3	1.95	0.48
1:A:42:LEU:HD12	1:A:42:LEU:H	1.77	0.48
1:A:316:LYS:HE3	1:A:316:LYS:HB2	1.78	0.48
1:A:636:ILE:HD13	1:A:851:ILE:CD1	2.44	0.48
1:A:616:CYS:SG	1:A:617:PRO:CD	3.00	0.48
1:A:411:GLU:HB3	1:A:413:LEU:HG	1.95	0.48
1:A:358:TRP:CE2	1:A:359:MET:HG3	2.49	0.48
1:A:626:ASP:HB2	1:A:826:ASN:HD22	1.78	0.48
1:A:376:LEU:HD21	1:A:512:TYR:CE1	2.49	0.47
1:A:243:THR:HG22	1:A:246:ASP:N	2.29	0.47
1:A:13:LYS:HA	1:A:102:ASN:HD22	1.79	0.47
1:A:26:VAL:HA	1:A:29:VAL:HG12	1.96	0.47
1:A:610:ALA:HB2	1:A:622:LEU:HD23	1.96	0.47
1:A:62:LEU:O	1:A:76:LEU:HA	2.14	0.47
1:A:566:VAL:HB	3:A:861:4HM:HC3	1.96	0.47
1:A:581:TYR:O	1:A:585:MET:HG3	2.15	0.47
1:A:620:ILE:HD11	1:A:634:LEU:HD21	1.97	0.47
1:A:423:ARG:HH22	1:A:458:ASN:HD21	1.63	0.47
1:A:398:THR:HB	1:A:399:SER:H	1.32	0.46
1:A:775:ARG:HG3	1:A:845:GLY:CA	2.45	0.46
1:A:300:GLU:HG2	4:A:1122:HOH:O	2.15	0.46
1:A:380:LEU:O	1:A:381:LYS:HE2	2.15	0.46
1:A:473:HIS:HB2	1:A:476:GLY:C	2.36	0.46
1:A:785:GLU:CG	1:A:805:GLY:HA3	2.46	0.46
1:A:13:LYS:HA	1:A:102:ASN:ND2	2.31	0.46
1:A:168:LEU:CD2	1:A:169:PRO:HD2	2.46	0.46
1:A:164:ASN:HB3	1:A:793:SER:HB3	1.97	0.46
1:A:168:LEU:O	1:A:170:SER:N	2.48	0.46
1:A:635:GLU:HB3	1:A:811:ILE:HD12	1.97	0.46
1:A:214:ASP:OD1	1:A:243:THR:HG23	2.16	0.45
1:A:736:GLU:O	1:A:742:TYR:HB2	2.16	0.45
1:A:41:ASP:O	1:A:42:LEU:C	2.54	0.45
1:A:326:SER:H	1:A:327:PRO:CD	2.21	0.45
1:A:783:LEU:HA	1:A:853:ASN:OD1	2.15	0.45
1:A:78:LYS:HG3	4:A:1002:HOH:O	2.17	0.45
1:A:441:ASN:HD21	1:A:447:ALA:N	1.87	0.45
1:A:402:THR:HG23	1:A:485:VAL:HG11	1.99	0.45
1:A:10:HIS:CG	1:A:11:LYS:N	2.85	0.45
1:A:277:LEU:HG	1:A:772:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ASP:O	1:A:628:PRO:HD3	2.17	0.45
1:A:160:ILE:HG22	1:A:183:GLU:HG3	1.99	0.44
1:A:260:ARG:O	1:A:261:ASP:CB	2.65	0.44
1:A:190:ASP:CG	1:A:191:GLY:H	2.20	0.44
1:A:38:GLN:HB2	4:A:951:HOH:O	2.17	0.44
1:A:76:LEU:H	1:A:76:LEU:CD2	2.26	0.44
1:A:174:ALA:HB3	1:A:175:PRO:HD3	2.00	0.44
1:A:507:VAL:CG1	1:A:577:LEU:HD13	2.48	0.44
1:A:636:ILE:O	1:A:640:ILE:HG13	2.18	0.44
1:A:814:LYS:HE2	1:A:818:ARG:HH21	1.83	0.44
1:A:566:VAL:HB	3:A:861:4HM:C11	2.47	0.44
1:A:72:GLY:O	1:A:175:PRO:HA	2.18	0.43
1:A:333:GLU:HB3	4:A:1251:HOH:O	2.17	0.43
1:A:843:LYS:HG3	1:A:844:GLU:H	1.83	0.43
1:A:260:ARG:HA	1:A:260:ARG:HD2	1.83	0.43
1:A:13:LYS:HB2	1:A:133:GLU:HB2	2.00	0.43
1:A:717:TYR:CE1	1:A:771:GLU:HG3	2.53	0.43
1:A:275:TYR:HE2	1:A:329:PRO:HG2	1.83	0.43
1:A:350:VAL:O	1:A:831:VAL:HG23	2.19	0.43
1:A:311:TYR:CD2	4:A:921:HOH:O	2.69	0.43
1:A:318:PRO:HG2	1:A:321:ILE:CG1	2.41	0.43
1:A:775:ARG:HB2	1:A:775:ARG:HH11	1.83	0.43
1:A:118:LYS:HD2	4:A:1273:HOH:O	2.19	0.43
1:A:297:THR:HG21	1:A:315:ILE:HD11	2.01	0.43
1:A:518:HIS:HE1	3:A:861:4HM:C5	2.32	0.43
1:A:717:TYR:HB3	1:A:718:PRO:HD3	2.01	0.43
1:A:189:GLY:O	1:A:190:ASP:HB3	2.19	0.42
1:A:564:SER:HA	1:A:567:ASN:OD1	2.18	0.42
1:A:169:PRO:HB2	1:A:662:PRO:HD2	2.01	0.42
1:A:317:LEU:HB3	1:A:318:PRO:HD2	2.01	0.42
1:A:440:ILE:HD11	1:A:585:MET:HE1	2.00	0.42
1:A:762:GLN:HE21	1:A:762:GLN:H	1.64	0.42
1:A:775:ARG:HB2	1:A:775:ARG:NH1	2.33	0.42
1:A:788:ASN:CB	1:A:789:PRO:HD3	2.29	0.42
1:A:557:ILE:O	1:A:557:ILE:HD13	2.19	0.42
1:A:147:SER:OG	1:A:159:ARG:NH2	2.52	0.42
1:A:387:SER:HB3	1:A:395:GLY:CA	2.40	0.42
1:A:438:ARG:NE	1:A:473:HIS:HE1	2.18	0.42
1:A:169:PRO:HD3	1:A:541:HIS:CE1	2.54	0.42
1:A:340:GLU:CG	1:A:341:GLN:HG3	2.49	0.42
1:A:594:VAL:HG13	4:A:954:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:THR:CG2	1:A:849:ARG:HG2	2.41	0.42
1:A:89:LEU:HA	1:A:90:PRO:HD3	1.84	0.41
1:A:311:TYR:HB3	1:A:345:PHE:O	2.20	0.41
1:A:386:ARG:HB3	1:A:398:THR:CG2	2.43	0.41
1:A:660:GLU:O	1:A:662:PRO:HD3	2.19	0.41
1:A:252:ARG:NH2	1:A:562:ARG:O	2.54	0.41
1:A:785:GLU:CD	1:A:805:GLY:HA3	2.41	0.41
1:A:136:PRO:C	1:A:138:HIS:H	2.23	0.41
1:A:493:VAL:O	1:A:497:ILE:HG13	2.19	0.41
1:A:631:VAL:HG12	1:A:818:ARG:NH1	2.36	0.41
1:A:728:THR:HG22	4:A:1174:HOH:O	2.21	0.41
1:A:155:PHE:O	1:A:156:LYS:HB3	2.20	0.41
1:A:336:ARG:HB3	1:A:344:LYS:HB2	2.02	0.41
1:A:328:LEU:HD12	1:A:328:LEU:N	2.35	0.41
1:A:42:LEU:C	1:A:44:GLY:H	2.23	0.41
1:A:611:ILE:HG12	1:A:621:ARG:HB3	2.03	0.41
1:A:269:SER:O	1:A:330:VAL:HG22	2.20	0.41
1:A:11:LYS:CG	1:A:102:ASN:HB3	2.50	0.41
1:A:134:ASP:OD2	1:A:138:HIS:HB3	2.21	0.41
1:A:195:ARG:HA	1:A:195:ARG:HD3	1.90	0.41
1:A:317:LEU:O	1:A:341:GLN:HG2	2.20	0.41
1:A:427:LEU:HB3	1:A:452:THR:HG23	2.01	0.41
1:A:381:LYS:HE2	1:A:381:LYS:CA	2.49	0.40
1:A:394:TYR:CA	1:A:397:HIS:HB3	2.51	0.40
1:A:762:GLN:NE2	1:A:762:GLN:N	2.69	0.40
1:A:40:LEU:HD22	1:A:40:LEU:HA	1.96	0.40
1:A:168:LEU:C	1:A:170:SER:H	2.24	0.40
1:A:441:ASN:ND2	1:A:446:LYS:HA	2.37	0.40
1:A:65:ALA:HA	1:A:176:LEU:HD13	2.03	0.40
1:A:172:THR:O	1:A:173:PRO:C	2.59	0.40
1:A:593:TRP:O	1:A:679:LYS:HE2	2.22	0.40
1:A:62:LEU:HD22	1:A:62:LEU:N	2.36	0.40
1:A:347:PRO:HA	1:A:348:PRO:HD3	1.87	0.40
1:A:493:VAL:HG22	1:A:746:ARG:HG2	2.03	0.40
1:A:836:THR:HG22	1:A:836:THR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	847/857 (99%)	748 (88%)	66 (8%)	33 (4%)	3 1

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	78	LYS
1	A	134	ASP
1	A	172	THR
1	A	394	TYR
1	A	398	THR
1	A	408	PRO
1	A	477	ASP
1	A	481	ALA
1	A	784	GLY
1	A	789	PRO
1	A	261	ASP
1	A	295	ASN
1	A	393	VAL
1	A	397	HIS
1	A	411	GLU
1	A	135	ILE
1	A	137	ASN
1	A	169	PRO
1	A	326	SER
1	A	390	ASP
1	A	737	LYS
1	A	844	GLU
1	A	69	ASP
1	A	89	LEU
1	A	785	GLU
1	A	788	ASN
1	A	33	GLY

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Mol	Chain	Res	Type
1	A	407	GLU
1	A	101	ILE
1	A	473	HIS
1	A	72	GLY
1	A	330	VAL

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	743/749 (99%)	677 (91%)	66 (9%)	9 9

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	18	LEU
1	A	35	ILE
1	A	36	ILE
1	A	40	LEU
1	A	41	ASP
1	A	47	LEU
1	A	54	LEU
1	A	67	LYS
1	A	76	LEU
1	A	82	LEU
1	A	83	GLU
1	A	100	LYS
1	A	122	GLN
1	A	164	ASN
1	A	166	THR
1	A	176	LEU
1	A	183	GLU
1	A	187	LEU
1	A	198	TRP
1	A	208	ASN

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Mol	Chain	Res	Type
1	A	218	ASN
1	A	232	TYR
1	A	243	THR
1	A	296	PHE
1	A	300	GLU
1	A	311	TYR
1	A	316	LYS
1	A	328	LEU
1	A	351	ILE
1	A	390	ASP
1	A	398	THR
1	A	406	LEU
1	A	410	LEU
1	A	427	LEU
1	A	452	THR
1	A	465	LEU
1	A	485	VAL
1	A	522	THR
1	A	537	LEU
1	A	539	VAL
1	A	547	LEU
1	A	553	ASP
1	A	557	ILE
1	A	594	VAL
1	A	604	LEU
1	A	621	ARG
1	A	626	ASP
1	A	627	TYR
1	A	634	LEU
1	A	713	ASN
1	A	722	LEU
1	A	735	PRO
1	A	737	LYS
1	A	747	LYS
1	A	754	LEU
1	A	773	LEU
1	A	787	ASP
1	A	798	LEU
1	A	808	LEU
1	A	815	LEU
1	A	822	GLU
1	A	825	ARG

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Mol	Chain	Res	Type
1	A	832	GLN
1	A	837	LEU
1	A	838	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	96	GLN
1	A	102	ASN
1	A	122	GLN
1	A	164	ASN
1	A	186	ASN
1	A	208	ASN
1	A	282	GLN
1	A	289	GLN
1	A	397	HIS
1	A	400	GLN
1	A	441	ASN
1	A	458	ASN
1	A	473	HIS
1	A	508	ASN
1	A	521	ASN
1	A	541	HIS
1	A	556	ASN
1	A	618	HIS
1	A	665	GLN
1	A	725	ASN
1	A	750	GLN
1	A	762	GLN
1	A	819	ASN
1	A	820	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
3	4HM	A	861	2	10,11,11	0.94	0	13,14,14	2.32	2 (15%)

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	4HM	A	861	2	-	2/2/4/4	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	861	4HM	C11-O9-C2	7.79	129.28	117.53
3	A	861	4HM	O9-C2-C1	2.46	118.13	114.57

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	861	4HM	C3-C2-O9-C11
3	A	861	4HM	C1-C2-O9-C11

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	861	4HM	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	849/857 (99%)	-0.07	51 (6%)	21	20	9, 30, 85, 100	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	GLY	9.4
1	A	43	VAL	9.0
1	A	34	GLY	8.7
1	A	46	THR	8.4
1	A	45	SER	8.4
1	A	410	LEU	7.9
1	A	31	SER	7.4
1	A	41	ASP	7.0
1	A	32	VAL	6.8
1	A	40	LEU	6.8
1	A	784	GLY	6.5
1	A	135	ILE	6.2
1	A	409	ASN	6.1
1	A	393	VAL	5.5
1	A	39	GLY	5.3
1	A	36	ILE	5.2
1	A	47	LEU	4.8
1	A	396	ASP	4.5
1	A	296	PHE	4.2
1	A	395	GLY	4.1
1	A	411	GLU	4.1
1	A	9	GLY	3.8
1	A	42	LEU	3.8
1	A	38	GLN	3.6
1	A	35	ILE	3.5
1	A	107	ASP	3.5
1	A	337	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	394	TYR	3.2
1	A	405	HIS	3.2
1	A	37	GLY	3.2
1	A	33	GLY	3.2
1	A	397	HIS	3.1
1	A	48	ASP	3.1
1	A	789	PRO	3.0
1	A	30	THR	2.9
1	A	342	ALA	2.9
1	A	71	ASN	2.8
1	A	340	GLU	2.7
1	A	788	ASN	2.7
1	A	785	GLU	2.7
1	A	137	ASN	2.5
1	A	398	THR	2.5
1	A	72	GLY	2.5
1	A	171	GLU	2.5
1	A	737	LYS	2.3
1	A	408	PRO	2.3
1	A	739	SER	2.2
1	A	616	CYS	2.2
1	A	83	GLU	2.1
1	A	325	ILE	2.0
1	A	336	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	4HM	A	861	11/11	0.91	0.30	42,64,71,73	0
2	FE	A	858	1/1	0.95	0.06	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.