



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:45 AM UTC

PDB ID : 2B3Y / pdb_00002b3y
Title : Structure of a monoclinic crystal form of human cytosolic aconitase (IRP1)
Authors : Dupuy, J.; Fontecilla-Camps, J.C.; Volbeda, A.
Deposited on : 2005-09-22
Resolution : 1.85 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

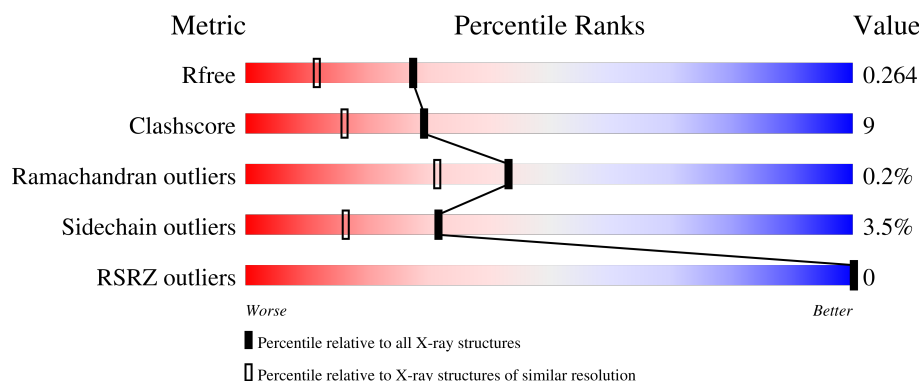
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	888	
1	B	888	

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	ACT	A	890	-	-	X	-
2	ACT	B	890	-	-	X	-
2	ACT	B	891	-	-	X	-
5	FMT	B	1001	-	-	X	-

2 Entry composition [i](#)

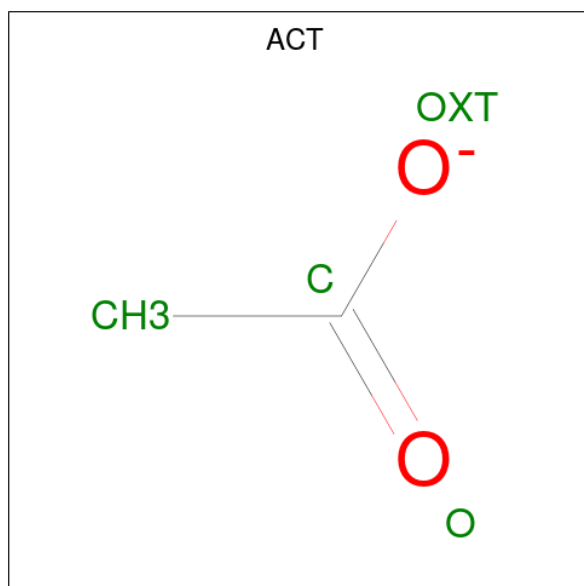
There are 6 unique types of molecules in this entry. The entry contains 14870 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Iron-responsive element binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	888	Total	C	N	O	S	0	1	0
			6929	4431	1183	1286	29			
1	B	888	Total	C	N	O	S	0	0	0
			6928	4431	1183	1285	29			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			3	1	2		

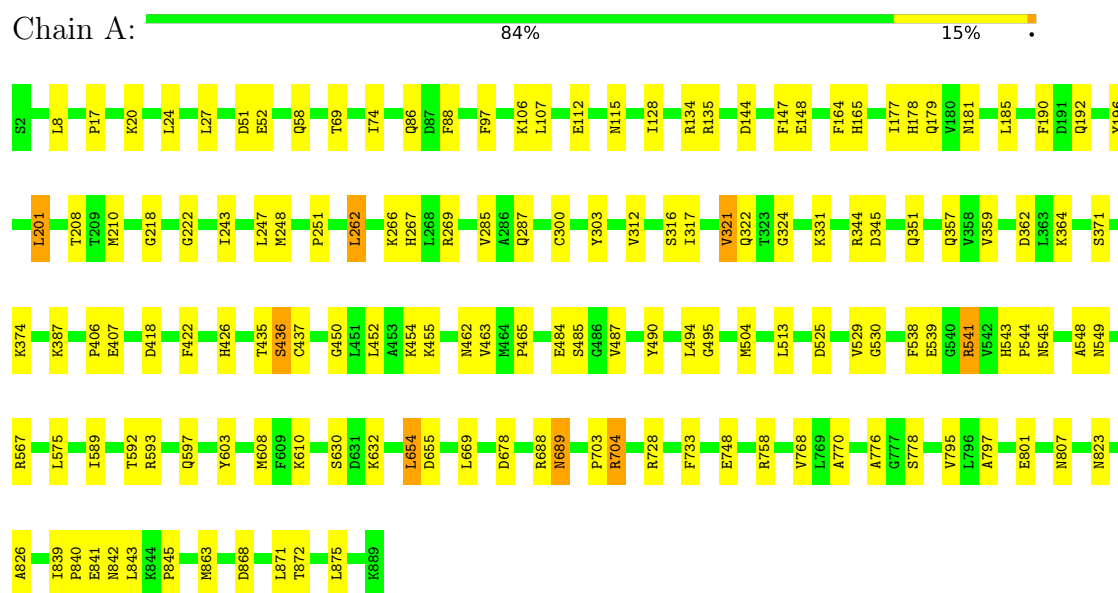
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	520	Total	O	0	0
			520	520		
6	B	450	Total	O	0	0
			450	450		

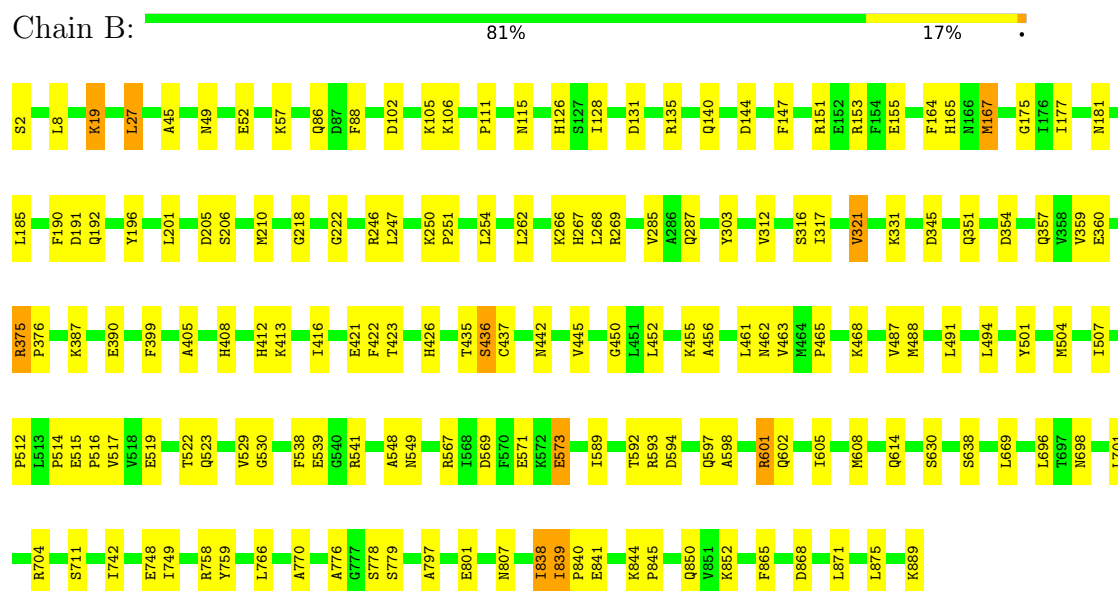
3 Residue-property plots

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: Iron-responsive element binding protein 1



- Molecule 1: Iron-responsive element binding protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.91Å 215.47Å 64.01Å 90.00° 72.00° 90.00°	Depositor
Resolution (Å)	29.50 – 1.85 29.50 – 1.85	Depositor EDS
% Data completeness (in resolution range)	94.0 (29.50-1.85) 98.8 (29.50-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.211 , 0.261 0.214 , 0.264	Depositor DCC
R_{free} test set	6949 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.408 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14870	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, SF4, FMT, GOL

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	0.69	0/7095	0.88	3/9634 (0.0%)
1	B	0.68	0/7089	0.87	5/9626 (0.1%)
All	All	0.68	0/14184	0.87	8/19260 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	839	ILE	CA-C-N	6.69	126.65	120.03
1	B	839	ILE	C-N-CA	6.69	126.65	120.03
1	A	179	GLN	N-CA-C	-6.24	104.01	111.69
1	A	300	CYS	CA-C-N	-5.92	113.58	119.56
1	A	300	CYS	C-N-CA	-5.92	113.58	119.56
1	B	605	ILE	CA-C-N	5.84	125.98	119.32
1	B	605	ILE	C-N-CA	5.84	125.98	119.32
1	B	268	LEU	N-CA-C	5.04	117.67	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6929	0	6921	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6928	0	6920	120	0
2	A	4	0	3	2	0
2	B	8	0	6	11	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	12	0	16	1	0
5	B	3	0	1	10	0
6	A	520	0	0	21	0
6	B	450	0	0	16	0
All	All	14870	0	13867	239	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 9.

All (239) 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)
2:B:891:ACT:CH3	5:B:1001:FMT:H	1.72	1.17
1:B:450:GLY:HA3	1:B:487:VAL:HG11	1.33	1.09
1:A:450:GLY:HA3	1:A:487:VAL:HG11	1.36	1.08
1:B:450:GLY:CA	1:B:487:VAL:HG11	1.85	1.06
1:A:450:GLY:CA	1:A:487:VAL:HG11	1.85	1.05
2:B:891:ACT:CH3	5:B:1001:FMT:C	2.37	1.03
2:B:891:ACT:H3	5:B:1001:FMT:H	1.41	0.98
2:B:890:ACT:H2	2:B:891:ACT:H2	1.46	0.94
1:A:222:GLY:HA3	1:A:807:ASN:HD21	1.35	0.91
2:B:891:ACT:H2	5:B:1001:FMT:H	1.50	0.91
1:B:345:ASP:H	1:B:351:GLN:HE22	1.22	0.83
1:B:222:GLY:HA3	1:B:807:ASN:HD21	1.45	0.82
2:B:891:ACT:H2	5:B:1001:FMT:C	2.05	0.81
1:B:845:PRO:HD3	6:B:1384:HOH:O	1.80	0.80
1:A:539:GLU:HG3	1:A:728:ARG:HD3	1.62	0.79
1:B:838:ILE:HD11	1:B:852:LYS:HD3	1.65	0.77
1:B:748:GLU:OE1	1:B:758:ARG:NH1	2.16	0.77
1:B:102:ASP:O	1:B:106:LYS:HG2	1.85	0.76
1:A:135:ARG:NH2	6:A:1104:HOH:O	2.18	0.76
2:B:890:ACT:H2	2:B:891:ACT:CH3	2.16	0.76
1:B:450:GLY:CA	1:B:487:VAL:CG1	2.65	0.74
1:B:598:ALA:O	1:B:602:GLN:HG2	1.88	0.73
1:A:450:GLY:C	1:A:487:VAL:HG11	2.13	0.73
1:A:345:ASP:H	1:A:351:GLN:HE22	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLU:OE2	1:A:632:LYS:HD2	1.87	0.72
1:B:450:GLY:C	1:B:487:VAL:HG11	2.15	0.72
1:A:842:ASN:HB3	6:A:1519:HOH:O	1.90	0.72
1:A:58:GLN:OE1	6:A:1017:HOH:O	2.08	0.71
1:A:251:PRO:O	1:A:593:ARG:NH2	2.22	0.71
1:B:375:ARG:HD3	1:B:399:PHE:CD2	2.26	0.71
1:B:865:PHE:HB2	1:B:871:LEU:HD23	1.72	0.71
1:B:593:ARG:HG2	1:B:597:GLN:NE2	2.06	0.70
1:B:742:ILE:HG12	1:B:749:ILE:CD1	2.22	0.70
1:B:865:PHE:CB	1:B:871:LEU:HD23	2.22	0.70
1:A:841:GLU:HB3	6:A:1416:HOH:O	1.93	0.69
1:B:742:ILE:HG12	1:B:749:ILE:HD12	1.75	0.69
1:B:698:ASN:ND2	6:B:1315:HOH:O	2.27	0.67
1:B:779:SER:H	5:B:1001:FMT:C	2.08	0.66
1:A:324:GLY:O	1:A:610:LYS:HE3	1.95	0.66
1:A:344:ARG:HH11	1:A:351:GLN:HE21	1.44	0.65
1:B:421:GLU:OE1	1:B:421:GLU:N	2.29	0.65
4:A:1001:GOL:H2	6:A:1194:HOH:O	1.95	0.65
1:A:733:PHE:O	6:A:1365:HOH:O	2.14	0.65
1:A:454:LYS:HD2	1:A:490:TYR:CE1	2.33	0.64
1:B:357:GLN:OE1	6:B:1148:HOH:O	2.15	0.64
1:A:422:PHE:CZ	1:A:465:PRO:HD2	2.33	0.64
1:B:455:LYS:CB	1:B:589:ILE:HG23	2.29	0.63
1:A:776:ALA:HA	1:A:801:GLU:HG3	1.81	0.63
1:A:262:LEU:HG	1:A:371:SER:OG	1.97	0.63
1:A:455:LYS:HD2	1:A:589:ILE:HA	1.80	0.62
1:A:450:GLY:CA	1:A:487:VAL:CG1	2.70	0.62
1:A:655:ASP:OD2	6:A:1345:HOH:O	2.16	0.62
1:B:838:ILE:HD12	1:B:838:ILE:N	2.16	0.61
1:B:205:ASP:HA	5:B:1001:FMT:O1	2.00	0.60
1:B:115:ASN:ND2	1:B:165:HIS:H	1.99	0.60
1:B:375:ARG:NH1	6:B:1199:HOH:O	2.22	0.60
1:B:569:ASP:OD2	1:B:571:GLU:HG2	2.00	0.60
1:A:107:LEU:HD13	1:A:654:LEU:HD13	1.84	0.60
1:B:456:ALA:HA	1:B:589:ILE:HD13	1.82	0.60
2:B:891:ACT:H3	5:B:1001:FMT:C	2.21	0.60
1:B:131:ASP:O	6:B:1057:HOH:O	2.17	0.59
1:B:461:LEU:HD12	1:B:589:ILE:CD1	2.32	0.59
1:A:267:HIS:CE1	1:A:359:VAL:CG1	2.86	0.58
1:B:405:ALA:HB3	1:B:408:HIS:HD2	1.67	0.58
1:B:455:LYS:HB3	1:B:589:ILE:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:GLU:CD	1:A:758:ARG:HH12	2.12	0.58
1:B:52:GLU:OE1	1:B:57:LYS:N	2.36	0.58
1:B:267:HIS:CE1	1:B:359:VAL:CG1	2.87	0.58
1:A:247:LEU:HD12	1:A:285:VAL:HG22	1.85	0.57
2:B:890:ACT:CH3	2:B:891:ACT:H2	2.29	0.57
1:A:106:LYS:HD2	6:A:1092:HOH:O	2.05	0.57
1:A:192:GLN:HE22	1:B:630:SER:HB2	1.70	0.56
1:A:688:ARG:CZ	1:A:703:PRO:HG2	2.35	0.56
1:B:345:ASP:H	1:B:351:GLN:NE2	1.96	0.56
1:B:201:LEU:O	1:B:218:GLY:HA2	2.06	0.56
1:A:115:ASN:ND2	1:A:165:HIS:H	2.04	0.56
1:B:450:GLY:C	1:B:487:VAL:CG1	2.79	0.56
1:B:488:MET:HE3	1:B:491:LEU:HB2	1.87	0.56
1:A:322:GLN:NE2	6:A:1161:HOH:O	2.39	0.55
1:B:106:LYS:HD3	1:B:106:LYS:N	2.21	0.55
1:A:778:SER:OG	2:A:890:ACT:H3	2.06	0.55
1:B:416:ILE:O	1:B:416:ILE:HG13	2.07	0.55
1:A:17:PRO:O	1:A:20:LYS:HE3	2.07	0.54
1:B:206:SER:N	5:B:1001:FMT:O1	2.33	0.54
1:A:823:ASN:ND2	1:A:826:ALA:H	2.04	0.54
1:B:529:VAL:HG22	1:B:548:ALA:HB3	1.89	0.54
1:A:454:LYS:NZ	6:A:1229:HOH:O	2.41	0.54
1:B:19:LYS:HE2	1:B:191:ASP:OD1	2.08	0.53
1:A:748:GLU:OE2	1:A:758:ARG:NH2	2.41	0.53
1:A:248:MET:HG3	1:A:362:ASP:HA	1.91	0.53
1:A:529:VAL:HG22	1:A:548:ALA:HB3	1.89	0.53
1:A:487:VAL:HG12	1:A:487:VAL:O	2.09	0.53
1:A:539:GLU:HG2	6:A:1204:HOH:O	2.09	0.53
1:A:593:ARG:HD3	1:A:597:GLN:OE1	2.09	0.52
1:B:776:ALA:HA	1:B:801:GLU:HG3	1.91	0.52
1:B:251:PRO:O	1:B:593:ARG:NH1	2.41	0.52
1:B:105:LYS:HB2	1:B:111:PRO:HG3	1.91	0.52
1:A:688:ARG:NH2	1:A:703:PRO:HG2	2.24	0.52
1:B:597:GLN:O	1:B:601:ARG:HB2	2.09	0.52
1:A:190:PHE:O	1:A:196:TYR:HA	2.10	0.51
1:A:243:ILE:HD12	1:A:357:GLN:HG2	1.92	0.51
1:B:140:GLN:NE2	1:B:144:ASP:OD1	2.43	0.51
1:B:375:ARG:HD3	1:B:399:PHE:CG	2.45	0.51
1:B:541:ARG:O	1:B:541:ARG:HG2	2.09	0.51
1:A:450:GLY:C	1:A:487:VAL:CG1	2.82	0.51
1:A:374:LYS:HE2	6:A:1231:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ARG:HB3	1:B:360:GLU:HG2	1.93	0.50
1:B:269:ARG:HG2	1:B:303:TYR:HA	1.93	0.50
1:B:210:MET:HE1	1:B:437:CYS:O	2.12	0.50
1:B:450:GLY:O	1:B:487:VAL:HG13	2.11	0.50
1:A:222:GLY:HA3	1:A:807:ASN:ND2	2.16	0.50
1:B:541:ARG:NH2	6:B:1180:HOH:O	2.45	0.50
1:A:406:PRO:HD2	1:A:407:GLU:OE2	2.11	0.50
1:B:126:HIS:NE2	2:B:890:ACT:H1	2.27	0.50
1:A:454:LYS:HD2	1:A:490:TYR:CZ	2.46	0.49
1:A:543:HIS:HE1	1:A:545:ASN:HD22	1.60	0.49
1:B:190:PHE:O	1:B:196:TYR:HA	2.11	0.49
1:A:251:PRO:HG2	1:A:593:ARG:HH21	1.77	0.49
1:B:696:LEU:HD22	1:B:701:LEU:HD12	1.94	0.49
1:B:455:LYS:HD2	1:B:589:ILE:O	2.11	0.49
1:A:484:GLU:HG3	1:A:608:MET:HE2	1.93	0.49
1:A:435:THR:O	1:A:436:SER:HB3	2.12	0.49
1:A:128:ILE:HG12	1:A:504:MET:HE3	1.95	0.49
1:B:569:ASP:O	1:B:573:GLU:HG3	2.12	0.49
1:B:614:GLN:HG3	6:B:1242:HOH:O	2.12	0.49
1:B:770:ALA:O	1:B:797:ALA:HA	2.13	0.49
1:B:452:LEU:C	1:B:452:LEU:HD23	2.38	0.49
1:B:115:ASN:HD22	1:B:165:HIS:H	1.58	0.48
1:B:593:ARG:HG2	1:B:597:GLN:HE21	1.75	0.48
1:A:530:GLY:O	1:A:549:ASN:HA	2.14	0.48
1:B:865:PHE:HB2	1:B:871:LEU:CD2	2.43	0.48
1:A:768:VAL:HB	1:A:795:VAL:HG22	1.96	0.48
1:A:317:ILE:O	1:A:321:VAL:HG12	2.13	0.48
1:A:362:ASP:OD1	1:A:364:LYS:HG2	2.14	0.48
1:A:452:LEU:HD23	1:A:452:LEU:C	2.38	0.47
1:B:838:ILE:HD12	1:B:838:ILE:H	1.79	0.47
1:B:530:GLY:O	1:B:549:ASN:HA	2.14	0.47
1:B:778:SER:OG	2:B:891:ACT:H3	2.15	0.47
1:A:418:ASP:OD2	6:A:1247:HOH:O	2.20	0.47
1:B:507:ILE:O	1:B:507:ILE:HG13	2.15	0.47
1:B:8:LEU:HD11	1:B:27:LEU:CD1	2.45	0.47
1:A:843:LEU:HD22	1:A:863:MET:HE1	1.97	0.46
1:B:19:LYS:HD2	1:B:19:LYS:HA	1.52	0.46
1:A:69:THR:HB	1:A:74:ILE:HD12	1.98	0.46
1:A:539:GLU:HG3	1:A:728:ARG:CD	2.39	0.46
1:B:115:ASN:ND2	1:B:164:PHE:HA	2.31	0.46
1:B:345:ASP:N	1:B:351:GLN:HE22	2.02	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:O	1:A:218:GLY:HA2	2.15	0.45
1:B:435:THR:O	1:B:436:SER:CB	2.65	0.45
1:B:317:ILE:O	1:B:321:VAL:HG12	2.17	0.45
1:A:8:LEU:HD11	1:A:27:LEU:HD11	1.99	0.45
1:A:487:VAL:CG1	1:A:487:VAL:O	2.65	0.45
1:A:426:HIS:HB2	1:A:567:ARG:NH1	2.31	0.44
1:A:704:ARG:HG3	6:A:1500:HOH:O	2.17	0.44
1:A:689:ASN:OD1	1:A:689:ASN:N	2.47	0.44
1:A:287:GLN:HG2	6:A:1157:HOH:O	2.16	0.44
1:B:514:PRO:HG2	1:B:517:VAL:CG2	2.48	0.44
1:B:538:PHE:O	1:B:539:GLU:C	2.60	0.44
1:B:871:LEU:O	1:B:875:LEU:HG	2.17	0.44
1:A:450:GLY:O	1:A:487:VAL:HG13	2.17	0.44
1:A:704:ARG:CG	6:A:1500:HOH:O	2.66	0.44
1:B:312:VAL:HG13	1:B:316:SER:HB2	1.99	0.44
1:A:20:LYS:HD2	6:A:1024:HOH:O	2.16	0.44
1:A:344:ARG:HD2	1:A:351:GLN:NE2	2.33	0.44
1:A:463:VAL:HG23	1:A:494:LEU:HD22	1.99	0.44
1:A:839:ILE:HA	1:A:840:PRO:HD3	1.85	0.44
1:B:181:ASN:HA	1:B:185:LEU:HB2	1.99	0.44
1:B:507:ILE:HD12	1:B:541:ARG:NH2	2.33	0.44
1:A:845:PRO:HG3	1:A:871:LEU:HD12	2.00	0.43
1:B:778:SER:OG	5:B:1001:FMT:H	2.18	0.43
1:B:839:ILE:HA	1:B:840:PRO:HD3	1.80	0.43
1:B:593:ARG:O	1:B:597:GLN:HG3	2.18	0.43
1:A:840:PRO:HD2	1:A:843:LEU:CD2	2.48	0.43
1:B:455:LYS:HB2	1:B:589:ILE:HG23	1.99	0.43
1:A:269:ARG:HG2	1:A:303:TYR:HA	2.01	0.43
1:B:376:PRO:HD3	1:B:538:PHE:CE1	2.53	0.43
1:B:704:ARG:NH1	6:B:1272:HOH:O	2.52	0.43
1:A:192:GLN:HE22	1:B:630:SER:CB	2.31	0.43
1:B:602:GLN:HB3	6:B:1422:HOH:O	2.17	0.43
1:B:515:GLU:N	1:B:516:PRO:CD	2.82	0.43
1:A:776:ALA:CA	1:A:801:GLU:HG3	2.48	0.43
1:A:868:ASP:O	1:A:872:THR:HG23	2.18	0.43
1:B:461:LEU:CD1	1:B:589:ILE:CD1	2.96	0.43
1:A:575:LEU:CD1	1:A:589:ILE:HD11	2.49	0.43
1:A:51:ASP:O	1:A:52:GLU:HB2	2.19	0.43
1:B:463:VAL:HG23	1:B:494:LEU:HD22	2.01	0.43
1:B:106:LYS:HE2	6:B:1405:HOH:O	2.19	0.42
1:A:134:ARG:HG3	1:A:495:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HG12	1:B:504:MET:HE3	2.01	0.42
1:A:543:HIS:CG	1:A:544:PRO:HD2	2.54	0.42
1:A:97:PHE:HB3	1:A:164:PHE:CZ	2.55	0.42
1:A:115:ASN:HD21	1:A:164:PHE:HA	1.84	0.42
1:A:178:HIS:CE1	1:A:208:THR:HA	2.55	0.42
1:B:357:GLN:HB2	6:B:1155:HOH:O	2.18	0.42
1:B:254:LEU:HB2	6:B:1142:HOH:O	2.18	0.42
1:B:426:HIS:HB2	1:B:567:ARG:NH1	2.33	0.42
1:A:24:LEU:HA	1:A:27:LEU:HD13	2.02	0.42
1:A:513:LEU:HG	1:A:543:HIS:CE1	2.54	0.42
1:B:45:ALA:O	1:B:49:ASN:HB2	2.20	0.42
1:A:144:ASP:O	1:A:148:GLU:HG3	2.20	0.42
1:A:312:VAL:HG13	1:A:316:SER:HB2	2.02	0.42
1:A:407:GLU:H	1:A:407:GLU:CD	2.28	0.42
1:A:538:PHE:O	1:A:539:GLU:C	2.62	0.42
1:A:875:LEU:CD1	6:A:1496:HOH:O	2.68	0.42
1:B:175:GLY:HA2	1:B:501:TYR:HB3	2.02	0.42
1:B:222:GLY:HA3	1:B:807:ASN:ND2	2.24	0.42
1:A:210:MET:HE1	1:A:437:CYS:O	2.20	0.42
1:B:115:ASN:HD21	1:B:164:PHE:HA	1.85	0.42
1:A:267:HIS:HE1	1:A:359:VAL:CG1	2.32	0.41
1:A:465:PRO:HG2	6:A:1256:HOH:O	2.20	0.41
1:A:630:SER:HB2	1:B:192:GLN:HE22	1.85	0.41
1:A:704:ARG:HG3	1:A:704:ARG:H	1.47	0.41
1:A:8:LEU:HD11	1:A:27:LEU:CD1	2.50	0.41
1:B:140:GLN:HB2	6:B:1087:HOH:O	2.19	0.41
1:B:422:PHE:CZ	1:B:465:PRO:HD2	2.55	0.41
1:B:442:ASN:HB3	1:B:445:VAL:HG22	2.02	0.41
1:B:468:LYS:NZ	1:B:512:PRO:O	2.47	0.41
1:A:192:GLN:NE2	6:A:1070:HOH:O	2.53	0.41
1:A:770:ALA:O	1:A:797:ALA:HA	2.20	0.41
1:A:541:ARG:HA	1:A:541:ARG:HD2	1.90	0.41
1:A:845:PRO:HD3	6:A:1326:HOH:O	2.20	0.41
1:A:485:SER:HA	1:A:603:TYR:CZ	2.55	0.41
1:B:153:ARG:HD2	1:B:711:SER:O	2.21	0.41
1:B:247:LEU:HD12	1:B:285:VAL:HG22	2.01	0.41
1:B:106:LYS:CE	6:B:1405:HOH:O	2.69	0.41
1:B:167:MET:HB3	1:B:167:MET:HE3	1.80	0.41
1:B:151:ARG:O	1:B:155:GLU:HG3	2.21	0.41
1:B:19:LYS:HB3	1:B:196:TYR:CE2	2.56	0.41
1:B:450:GLY:HA3	1:B:487:VAL:CG1	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PHE:HB3	1:A:164:PHE:CE2	2.56	0.40
1:A:181:ASN:HA	1:A:185:LEU:HB2	2.02	0.40
1:A:115:ASN:HD22	1:A:165:HIS:H	1.69	0.40
1:A:778:SER:OG	2:A:890:ACT:CH3	2.69	0.40
1:B:412:HIS:HB2	1:B:423:THR:HG22	2.03	0.40
1:A:115:ASN:ND2	1:A:164:PHE:HA	2.35	0.40
1:B:594:ASP:HB2	6:B:1425:HOH:O	2.21	0.40
1:B:868:ASP:CG	6:B:1284:HOH:O	2.65	0.40
1:B:105:LYS:HG2	1:B:106:LYS:HD3	2.03	0.40
1:B:759:TYR:CG	1:B:766:LEU:HD21	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	887/888 (100%)	857 (97%)	28 (3%)	2 (0%)	43	31
1	B	886/888 (100%)	857 (97%)	27 (3%)	2 (0%)	43	31
All	All	1773/1776 (100%)	1714 (97%)	55 (3%)	4 (0%)	43	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	SER
1	B	436	SER
1	B	177	ILE
1	A	177	ILE

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	752/751 (100%)	734 (98%)	18 (2%)	43	28
1	B	751/751 (100%)	717 (96%)	34 (4%)	24	10
All	All	1503/1502 (100%)	1451 (96%)	52 (4%)	32	16

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	88	PHE
1	A	147	PHE
1	A	201	LEU
1	A	262	LEU
1	A	266	LYS
1	A	321	VAL
1	A	331	LYS
1	A	387	LYS
1	A	462	ASN
1	A	525	ASP
1	A	541	ARG
1	A	592	THR
1	A	654	LEU
1	A	669	LEU
1	A	678	ASP
1	A	689	ASN
1	A	704	ARG
1	B	2	SER
1	B	19	LYS
1	B	27	LEU
1	B	86	GLN
1	B	88	PHE
1	B	135	ARG
1	B	147	PHE
1	B	167	MET
1	B	250	LYS

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Mol	Chain	Res	Type
1	B	262	LEU
1	B	266	LYS
1	B	287	GLN
1	B	321	VAL
1	B	331	LYS
1	B	354	ASP
1	B	375	ARG
1	B	387	LYS
1	B	390	GLU
1	B	413	LYS
1	B	462	ASN
1	B	519	GLU
1	B	522	THR
1	B	523	GLN
1	B	573	GLU
1	B	592	THR
1	B	601	ARG
1	B	608	MET
1	B	638	SER
1	B	669	LEU
1	B	838	ILE
1	B	841	GLU
1	B	844	LYS
1	B	850	GLN
1	B	889	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	25	ASN
1	A	49	ASN
1	A	71	HIS
1	A	115	ASN
1	A	192	GLN
1	A	233	GLN
1	A	322	GLN
1	A	351	GLN
1	A	397	GLN
1	A	408	HIS
1	A	409	HIS
1	A	462	ASN

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Mol	Chain	Res	Type
1	A	493	GLN
1	A	523	GLN
1	A	545	ASN
1	A	549	ASN
1	A	602	GLN
1	A	807	ASN
1	A	823	ASN
1	A	850	GLN
1	B	16	GLN
1	B	25	ASN
1	B	115	ASN
1	B	140	GLN
1	B	143	GLN
1	B	162	GLN
1	B	165	HIS
1	B	192	GLN
1	B	233	GLN
1	B	322	GLN
1	B	351	GLN
1	B	357	GLN
1	B	397	GLN
1	B	408	HIS
1	B	462	ASN
1	B	493	GLN
1	B	545	ASN
1	B	549	ASN
1	B	597	GLN
1	B	602	GLN
1	B	651	ASN
1	B	698	ASN
1	B	807	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SF4	B	1000	2,6,1	0,12,12	-	-	-		
2	ACT	B	890	3	3,3,3	0.73	0	3,3,3	1.24	0
4	GOL	A	1002	-	5,5,5	0.35	0	5,5,5	0.25	0
3	SF4	A	1000	6,1	0,12,12	-	-	-		
2	ACT	A	890	-	3,3,3	1.02	0	3,3,3	1.42	0
4	GOL	A	1001	-	5,5,5	0.41	0	5,5,5	0.18	0
2	ACT	B	891	-	3,3,3	1.06	0	3,3,3	1.81	1 (33%)
5	FMT	B	1001	-	2,2,2	0.94	0	1,1,1	0.30	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	SF4	B	1000	2,6,1	-	-	0/6/5/5
3	SF4	A	1000	6,1	-	-	0/6/5/5
4	GOL	A	1001	-	-	4/4/4/4	-
4	GOL	A	1002	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	891	ACT	OXT-C-O	-2.49	112.80	122.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	GOL	O1-C1-C2-O2
4	A	1001	GOL	O1-C1-C2-C3
4	A	1001	GOL	C1-C2-C3-O3
4	A	1002	GOL	O1-C1-C2-O2
4	A	1002	GOL	O1-C1-C2-C3
4	A	1002	GOL	C1-C2-C3-O3
4	A	1001	GOL	O2-C2-C3-O3
4	A	1002	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	890	ACT	4	0
2	A	890	ACT	2	0
4	A	1001	GOL	1	0
2	B	891	ACT	10	0
5	B	1001	FMT	10	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	888/888 (100%)	-1.22	0 100 100	16, 26, 40, 58	7 (0%)
1	B	888/888 (100%)	-1.12	0 100 100	17, 26, 40, 58	7 (0%)
All	All	1776/1776 (100%)	-1.17	0 100 100	16, 26, 40, 58	14 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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(Å ²)	Q<0.9
4	GOL	A	1001	6/6	0.93	0.09	48,48,51,54	0
4	GOL	A	1002	6/6	0.95	0.08	50,51,53,54	0
2	ACT	A	890	4/4	0.98	0.05	26,29,31,31	0
2	ACT	B	890	4/4	0.98	0.05	19,30,31,33	0
2	ACT	B	891	4/4	0.99	0.05	22,22,24,26	0
3	SF4	B	1000	8/8	0.99	0.05	22,25,30,31	0
5	FMT	B	1001	3/3	0.99	0.04	28,28,30,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SF4	A	1000	8/8	1.00	0.03	21,22,25,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.