



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:29 AM UTC

PDB ID : 3FSG / pdb_00003fsg
Title : Crystal structure of alpha/beta superfamily hydrolase from *Oenococcus oeni* PSU-1
Authors : Nocek, B.; Bigelow, L.; Cobb, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2009-01-09
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

<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

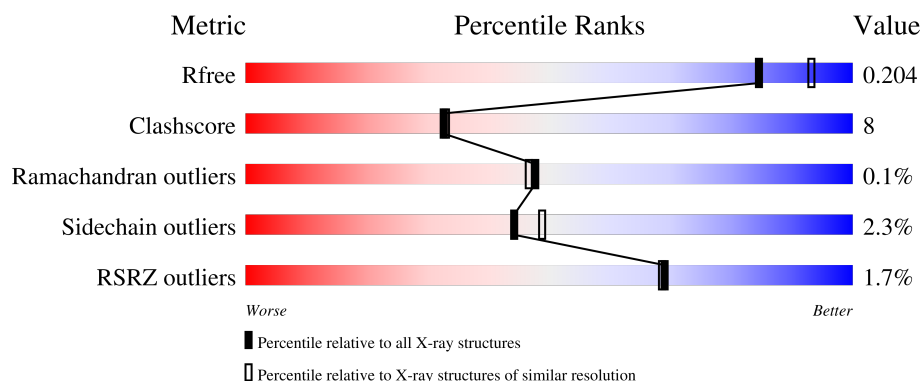
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	272	% 81% 15% ..
1	B	272	2% 78% 18% ..
1	C	272	% 80% 16% ..
2	D	272	2% 79% 17% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9199 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 Alpha/beta superfamily hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	Se	0	0	0
			2162	1385	359	411	2	5			
1	B	266	Total	C	N	O	S	Se	0	2	0
			2174	1392	363	412	2	5			
1	C	266	Total	C	N	O	S	Se	0	0	0
			2153	1379	358	409	2	5			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q04D10
A	-1	ASN	-	expression tag	UNP Q04D10
A	0	ALA	-	expression tag	UNP Q04D10
B	-2	SER	-	expression tag	UNP Q04D10
B	-1	ASN	-	expression tag	UNP Q04D10
B	0	ALA	-	expression tag	UNP Q04D10
C	-2	SER	-	expression tag	UNP Q04D10
C	-1	ASN	-	expression tag	UNP Q04D10
C	0	ALA	-	expression tag	UNP Q04D10

- Molecule 2 is a protein called Alpha/beta superfamily hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	264	Total	C	N	O	S	Se	0	1	0
			2141	1373	355	407	2	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP Q04D10
D	-1	ASN	-	expression tag	UNP Q04D10
D	0	ALA	-	expression tag	UNP Q04D10

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- 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	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		

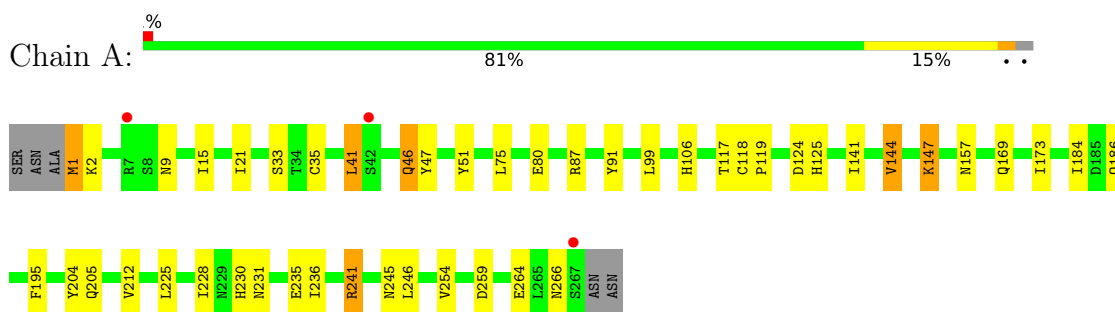
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	141	Total	O	0	0
			141	141		
7	B	125	Total	O	0	0
			125	125		
7	C	128	Total	O	0	0
			128	128		
7	D	98	Total	O	0	0
			98	98		

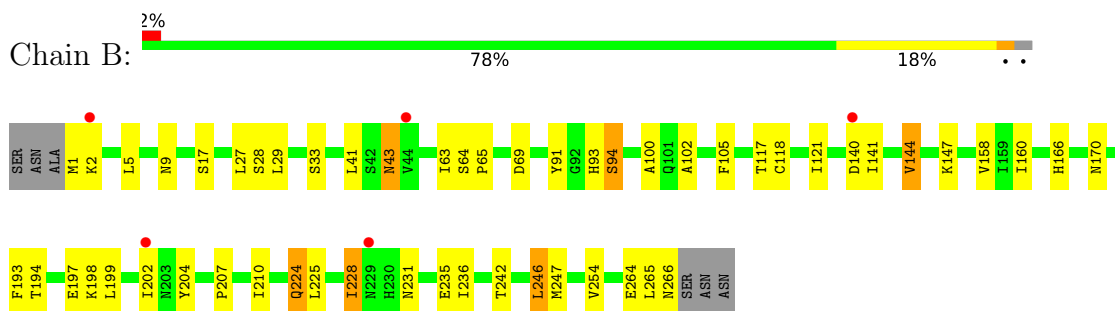
3 Residue-property plots [i](#)

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.

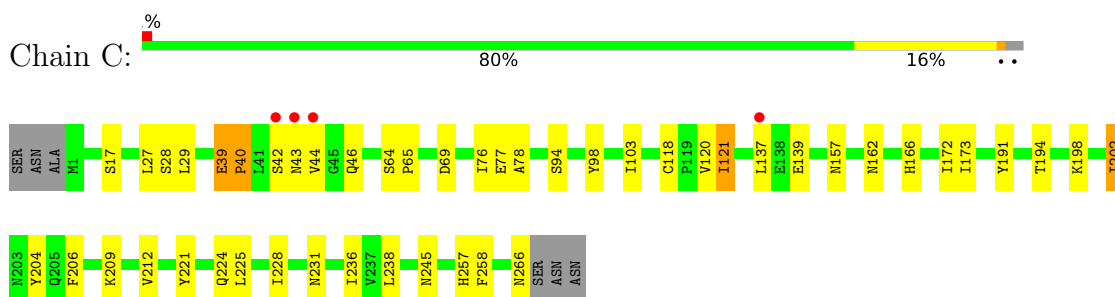
- Molecule 1: Alpha/beta superfamily hydrolase



- Molecule 1: Alpha/beta superfamily hydrolase

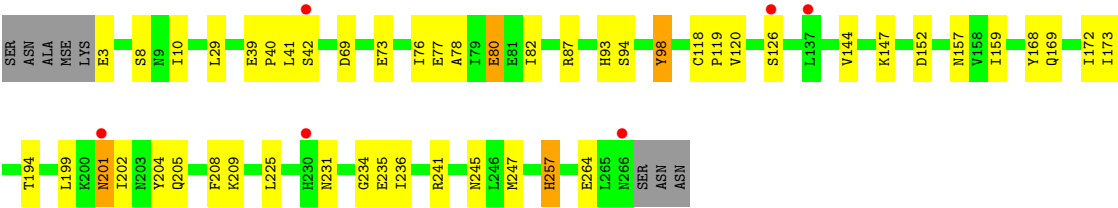


- Molecule 1: Alpha/beta superfamily hydrolase



- Molecule 2: Alpha/beta superfamily hydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	217.49Å 40.58Å 135.98Å 90.00° 107.50° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 40.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-2.00) 99.6 (40.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.180 , 0.225 0.198 , 0.204	Depositor DCC
R_{free} test set	3892 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.791	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9199	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, GOL, SO4, EDO, CL

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	1.30	5/2198 (0.2%)	1.10	2/2968 (0.1%)
1	B	1.31	11/2211 (0.5%)	1.04	1/2986 (0.0%)
1	C	1.34	7/2189 (0.3%)	1.09	9/2956 (0.3%)
2	D	1.20	1/2187 (0.0%)	1.04	2/2955 (0.1%)
All	All	1.29	24/8785 (0.3%)	1.07	14/11865 (0.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	118	CYS	C-O	-14.76	1.16	1.23
1	B	100	ALA	CA-CB	-8.16	1.40	1.53
1	B	94	SER	C-O	-7.72	1.17	1.24
1	B	33	SER	C-O	-6.33	1.16	1.24
1	A	33	SER	C-O	-6.31	1.16	1.24
1	B	254	VAL	C-O	-6.30	1.17	1.24
1	A	186	GLN	C-O	-6.12	1.17	1.24
1	C	76	ILE	C-O	-6.04	1.17	1.24
1	C	78	ALA	CA-CB	-5.66	1.44	1.53
1	C	103	ILE	C-O	-5.61	1.17	1.24
1	B	100	ALA	C-O	-5.46	1.17	1.24
1	C	39	GLU	C-O	-5.39	1.19	1.24
1	A	21	ILE	C-O	-5.37	1.18	1.24
1	B	63	ILE	C-O	-5.30	1.18	1.23
1	B	160	ILE	CA-CB	-5.29	1.47	1.53
1	C	77	GLU	C-O	-5.27	1.18	1.24
2	D	10	ILE	CA-CB	-5.22	1.48	1.54
1	A	51	TYR	C-O	-5.19	1.18	1.24
1	B	2	LYS	C-O	-5.09	1.17	1.23
1	B	246	LEU	C-O	-5.09	1.17	1.24
1	A	141	ILE	C-O	-5.06	1.18	1.24
1	B	29	LEU	C-O	-5.04	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	ILE	C-O	-5.03	1.19	1.24
1	C	94	SER	C-O	-5.01	1.17	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	121	ILE	CB-CA-C	-9.11	102.94	111.05
1	A	228	ILE	N-CA-C	8.19	118.23	110.53
1	C	43	ASN	N-CA-C	-6.86	101.25	111.81
1	C	173	ILE	N-CA-CB	6.57	114.64	110.50
2	D	257	HIS	N-CA-C	5.76	118.50	111.82
1	C	173	ILE	CA-C-N	-5.76	112.66	119.05
1	C	173	ILE	C-N-CA	-5.76	112.66	119.05
1	B	158	VAL	N-CA-C	-5.73	106.09	111.48
2	D	98	TYR	N-CA-C	-5.69	105.15	111.36
1	C	206	PHE	N-CA-C	-5.67	103.03	108.07
1	C	258	PHE	N-CA-C	-5.50	105.37	111.36
1	A	9	ASN	N-CA-C	5.26	118.64	111.39
1	C	202	ILE	CB-CA-C	-5.25	103.27	111.26
1	C	121	ILE	N-CA-C	-5.06	107.62	111.62

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	2162	0	2112	32	0
1	B	2174	0	2118	40	0
1	C	2153	0	2098	28	0
2	D	2141	0	2087	36	0
3	A	8	0	12	0	0
3	B	4	0	6	0	0
3	C	4	0	6	1	0
3	D	12	0	18	0	0
4	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	6	0	8	0	0
5	A	10	0	0	1	0
5	B	5	0	0	0	0
5	C	15	0	0	0	0
5	D	5	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	141	0	0	7	0
7	B	125	0	0	2	0
7	C	128	0	0	2	0
7	D	98	0	0	4	0
All	All	9199	0	8473	136	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 8.

All (136) 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:C:42:SER:HB2	1:C:44:VAL:HG22	1.35	1.06
1:B:144:VAL:HG13	7:B:361:HOH:O	1.68	0.93
1:C:42:SER:CB	1:C:44:VAL:HG22	2.04	0.86
2:D:199:LEU:HA	2:D:202:ILE:HD12	1.57	0.84
1:C:121:ILE:HD11	1:C:224:GLN:HG3	1.61	0.81
1:A:1:MSE:SE	1:A:15:ILE:HD11	2.33	0.78
1:B:224:GLN:HE21	1:B:224:GLN:H	1.33	0.75
1:C:69:ASP:OD2	1:C:194:THR:HG23	1.87	0.75
1:A:1:MSE:HE1	1:A:35:CSO:SG	2.28	0.74
2:D:157:ASN:ND2	2:D:245:ASN:HD22	1.85	0.74
1:B:105:PHE:CD1	1:B:202:ILE:HD11	2.26	0.71
1:B:5:LEU:HD21	1:B:9:ASN:OD1	1.92	0.69
2:D:93:HIS:CE1	2:D:247:MSE:HE1	2.29	0.68
2:D:144:VAL:O	2:D:147:LYS:HG3	1.95	0.67
1:B:224:GLN:H	1:B:224:GLN:NE2	1.93	0.67
2:D:204:TYR:H	2:D:231:ASN:HD21	1.41	0.67
1:A:1:MSE:SE	1:A:15:ILE:CD1	2.93	0.66
1:C:121:ILE:HD11	1:C:224:GLN:CG	2.24	0.66
2:D:69:ASP:OD2	2:D:194:THR:HG23	1.96	0.65
1:B:199:LEU:HA	1:B:202:ILE:HD12	1.79	0.65
1:B:121:ILE:HD11	1:B:224:GLN:HG3	1.78	0.65
1:C:266:ASN:C	7:C:347:HOH:O	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:TYR:H	3:C:2001:EDO:H22	1.64	0.62
2:D:199:LEU:HA	2:D:202:ILE:CD1	2.29	0.62
1:A:2:LYS:NZ	7:A:445:HOH:O	2.35	0.60
1:A:41:LEU:HD12	1:A:41:LEU:C	2.26	0.60
1:A:46:GLN:HG2	1:A:47:TYR:CD1	2.37	0.60
1:B:69:ASP:OD2	1:B:194:THR:HG23	2.02	0.60
1:C:204:TYR:H	1:C:231:ASN:HD21	1.49	0.59
1:B:105:PHE:CD1	1:B:202:ILE:CD1	2.85	0.59
1:B:41:LEU:HD13	1:B:43:ASN:ND2	2.17	0.59
1:B:235:GLU:OE1	1:B:264:GLU:OE1	2.20	0.59
2:D:159:ILE:HD11	2:D:241:ARG:HB3	1.85	0.59
2:D:204:TYR:H	2:D:231:ASN:ND2	2.01	0.59
1:C:157:ASN:ND2	1:C:245:ASN:HD22	2.01	0.58
1:A:87:ARG:NH1	7:A:270:HOH:O	2.29	0.58
1:C:212:VAL:HG23	1:C:238:LEU:HD13	1.86	0.57
1:A:157:ASN:ND2	1:A:245:ASN:HD22	2.02	0.57
1:B:198:LYS:O	1:B:202:ILE:HG13	2.05	0.57
1:C:204:TYR:H	1:C:231:ASN:ND2	2.02	0.56
2:D:144:VAL:HA	2:D:147:LYS:HE3	1.86	0.56
1:C:139:GLU:OE1	1:C:162:ASN:ND2	2.38	0.55
1:C:137:LEU:HD23	1:C:137:LEU:O	2.07	0.55
1:C:221:TYR:O	1:C:225:LEU:HD13	2.07	0.55
2:D:29:LEU:HD21	2:D:172:ILE:HG23	1.87	0.55
1:C:228:ILE:HG13	1:C:236:ILE:HB	1.87	0.55
2:D:209:LYS:NZ	2:D:257:HIS:HD1	2.04	0.55
1:A:230:HIS:HE1	7:A:344:HOH:O	1.89	0.54
1:B:93:HIS:CE1	1:B:247:MSE:HE1	2.42	0.54
1:A:241:ARG:HD2	7:A:317:HOH:O	2.08	0.54
1:B:102:ALA:HB2	1:B:193:PHE:CE2	2.43	0.54
2:D:199:LEU:HD23	2:D:202:ILE:CD1	2.39	0.53
2:D:169:GLN:HA	2:D:173:ILE:HD12	1.91	0.53
1:B:242:THR:HG21	1:B:246:LEU:HG	1.90	0.53
1:C:69:ASP:OD2	1:C:194:THR:CG2	2.57	0.53
2:D:118:CYS:N	2:D:119:PRO:CD	2.72	0.53
1:A:80:GLU:CG	7:A:337:HOH:O	2.57	0.52
1:A:41:LEU:HD13	1:A:259:ASP:OD1	2.10	0.52
1:B:225:LEU:HD12	1:B:236:ILE:HD13	1.92	0.52
2:D:225:LEU:HD23	2:D:236:ILE:HD13	1.91	0.52
2:D:94:SER:HA	2:D:118:CYS:O	2.11	0.51
1:B:210:ILE:HD12	1:B:228:ILE:HD11	1.93	0.51
1:C:137:LEU:HD23	1:C:137:LEU:C	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:ARG:HD2	7:D:416:HOH:O	2.11	0.50
1:C:225:LEU:HD12	1:C:236:ILE:HD13	1.93	0.50
1:B:140:ASP:O	1:B:140:ASP:OD1	2.30	0.49
2:D:3:GLU:N	7:D:355:HOH:O	2.45	0.49
2:D:93:HIS:NE2	2:D:247:MSE:HE1	2.27	0.49
1:C:98:TYR:HB2	1:C:120:VAL:HB	1.93	0.49
2:D:157:ASN:HD21	2:D:245:ASN:HD22	1.59	0.49
1:C:121:ILE:HD11	1:C:224:GLN:CD	2.38	0.48
2:D:208:PHE:O	2:D:234:GLY:HA2	2.13	0.48
1:C:39:GLU:N	1:C:40:PRO:HD2	2.28	0.48
2:D:209:LYS:HG3	2:D:235:GLU:HB2	1.96	0.48
2:D:78:ALA:O	2:D:82:ILE:HG13	2.14	0.48
2:D:98:TYR:HB2	2:D:120:VAL:HB	1.94	0.48
1:B:166[A]:HIS:O	1:B:170[A]:ASN:ND2	2.48	0.47
2:D:147:LYS:CD	7:D:307:HOH:O	2.61	0.47
2:D:152:ASP:OD2	2:D:168:TYR:OH	2.32	0.47
1:A:80:GLU:HG2	7:A:337:HOH:O	2.13	0.46
1:C:137:LEU:O	1:C:137:LEU:CD2	2.64	0.46
2:D:147:LYS:HD2	7:D:307:HOH:O	2.16	0.46
2:D:93:HIS:CE1	2:D:247:MSE:CE	2.98	0.46
2:D:201:ASN:N	2:D:201:ASN:OD1	2.48	0.46
1:A:117:THR:O	1:A:118:CYS:C	2.58	0.46
1:A:41:LEU:HD12	1:A:41:LEU:O	2.16	0.46
1:B:41:LEU:HD13	1:B:43:ASN:HD21	1.81	0.46
1:B:207:PRO:HG2	1:B:265:LEU:CD2	2.46	0.46
1:C:209:LYS:NZ	1:C:257:HIS:HD1	2.14	0.46
1:C:166:HIS:HB3	7:C:368:HOH:O	2.16	0.46
1:A:204:TYR:H	1:A:231:ASN:ND2	2.13	0.45
1:B:204:TYR:H	1:B:231:ASN:ND2	2.15	0.45
1:A:205:GLN:NE2	7:A:357:HOH:O	2.50	0.45
1:C:198:LYS:O	1:C:202:ILE:HG13	2.16	0.45
1:B:265:LEU:O	1:B:266:ASN:HB2	2.17	0.44
2:D:39:GLU:N	2:D:40:PRO:CD	2.81	0.44
1:B:242:THR:CG2	1:B:246:LEU:HG	2.48	0.44
2:D:73:GLU:O	2:D:77:GLU:HG3	2.17	0.44
1:C:27:LEU:O	1:C:28:SER:HB2	2.17	0.44
1:A:204:TYR:H	1:A:231:ASN:HD21	1.64	0.44
1:A:225:LEU:HD23	1:A:236:ILE:HD13	2.00	0.44
1:A:124:ASP:OD1	1:A:124:ASP:C	2.62	0.43
1:C:29:LEU:HD21	1:C:172:ILE:HG23	1.99	0.43
1:A:118:CYS:N	1:A:119:PRO:CD	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LEU:O	1:B:28:SER:HB2	2.18	0.43
1:C:64:SER:HA	1:C:65:PRO:C	2.43	0.43
1:A:169:GLN:HA	1:A:173:ILE:HD12	1.99	0.43
1:A:266:ASN:OD1	1:A:266:ASN:O	2.36	0.43
1:B:228:ILE:HG12	1:B:236:ILE:HB	2.01	0.43
1:A:246:LEU:CD2	1:A:254:VAL:CG2	2.97	0.43
1:A:106:HIS:HE1	1:A:195:PHE:CZ	2.37	0.43
1:B:64:SER:HA	1:B:65:PRO:C	2.43	0.43
1:B:207:PRO:HG2	1:B:265:LEU:HD23	1.99	0.43
1:A:144:VAL:O	1:A:147:LYS:HG3	2.19	0.42
1:B:140:ASP:OD1	1:B:140:ASP:C	2.60	0.42
1:A:91:TYR:CD2	1:A:91:TYR:C	2.97	0.42
1:B:94:SER:HA	1:B:118:CYS:O	2.19	0.42
1:B:210:ILE:HD12	1:B:228:ILE:CD1	2.48	0.42
1:A:246:LEU:HD23	1:A:254:VAL:CG2	2.49	0.42
1:B:5:LEU:CD2	1:B:9:ASN:OD1	2.66	0.42
1:B:117:THR:O	1:B:118:CYS:C	2.62	0.41
1:B:197:GLU:CD	1:B:197:GLU:H	2.27	0.41
2:D:76:ILE:HG23	2:D:80:GLU:OE2	2.20	0.41
1:B:144:VAL:O	1:B:147:LYS:HG3	2.20	0.41
1:B:246:LEU:C	1:B:246:LEU:HD23	2.45	0.41
2:D:235:GLU:OE1	2:D:264:GLU:OE1	2.38	0.41
2:D:205:GLN:NE2	2:D:205:GLN:HA	2.36	0.41
1:B:228:ILE:HG12	1:B:236:ILE:HD12	2.03	0.41
1:A:75:LEU:HD11	1:A:99:LEU:HD13	2.03	0.41
1:B:265:LEU:O	1:B:266:ASN:CB	2.69	0.41
1:B:91:TYR:CD2	1:B:91:TYR:C	2.99	0.40
2:D:82:ILE:HD13	2:D:82:ILE:HG21	1.86	0.40
1:A:118:CYS:SG	1:A:246:LEU:HB2	2.62	0.40
1:A:235:GLU:OE1	1:A:264:GLU:OE1	2.40	0.40
1:B:5:LEU:HD13	7:B:514:HOH:O	2.20	0.40
1:A:125:HIS:NE2	5:A:406:SO4:O3	2.54	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	264/272 (97%)	256 (97%)	8 (3%)	0	100	100
1	B	265/272 (97%)	256 (97%)	9 (3%)	0	100	100
1	C	263/272 (97%)	253 (96%)	9 (3%)	1 (0%)	30	27
2	D	263/272 (97%)	253 (96%)	10 (4%)	0	100	100
All	All	1055/1088 (97%)	1018 (96%)	36 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40	PRO

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	239/238 (100%)	231 (97%)	8 (3%)	33	34
1	B	240/238 (101%)	234 (98%)	6 (2%)	42	45
1	C	237/238 (100%)	235 (99%)	2 (1%)	73	80
2	D	238/239 (100%)	232 (98%)	6 (2%)	42	45
All	All	954/953 (100%)	932 (98%)	22 (2%)	44	49

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	41	LEU
1	A	46	GLN
1	A	144	VAL
1	A	147	LYS

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Mol	Chain	Res	Type
1	A	184	ILE
1	A	212	VAL
1	A	241	ARG
1	B	1	MSE
1	B	17	SER
1	B	43	ASN
1	B	144	VAL
1	B	224	GLN
1	B	228	ILE
1	C	17	SER
1	C	46	GLN
2	D	8	SER
2	D	41	LEU
2	D	42	SER
2	D	80	GLU
2	D	126	SER
2	D	201	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	106	HIS
1	A	110	GLN
1	A	157	ASN
1	A	163	GLN
1	A	177	GLN
1	A	201	ASN
1	A	205	GLN
1	A	215	ASN
1	A	222	GLN
1	A	230	HIS
1	A	231	ASN
1	B	43	ASN
1	B	46	GLN
1	B	70	ASN
1	B	163	GLN
1	B	177	GLN
1	B	201	ASN
1	B	205	GLN
1	B	224	GLN
1	B	231	ASN

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Mol	Chain	Res	Type
1	C	32	GLN
1	C	43	ASN
1	C	70	ASN
1	C	157	ASN
1	C	222	GLN
1	C	231	ASN
2	D	43	ASN
2	D	70	ASN
2	D	125	HIS
2	D	157	ASN
2	D	162	ASN
2	D	186	GLN
2	D	205	GLN
2	D	215	ASN
2	D	222	GLN
2	D	230	HIS
2	D	231	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSO	C	35	1	3,6,7	0.71	0	1,6,8	0.18	0
1	CSO	A	35	1	3,6,7	0.78	0	1,6,8	0.30	0
1	CSO	B	35	1	3,6,7	0.57	0	1,6,8	0.71	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
1	CSO	C	35	1	-	1/1/5/7	-
1	CSO	A	35	1	-	0/1/5/7	-
1	CSO	B	35	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	35	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	35	CSO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	GOL	D	3002	-	5,5,5	0.42	0	5,5,5	0.72	0
3	EDO	A	1003	-	3,3,3	0.46	0	2,2,2	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	3002	-	5,5,5	0.60	0	5,5,5	0.86	0
5	SO4	C	405	-	4,4,4	0.21	0	6,6,6	0.56	0
3	EDO	C	2001	-	3,3,3	0.52	0	2,2,2	0.71	0
3	EDO	A	1001	-	3,3,3	0.26	0	2,2,2	0.75	0
5	SO4	D	403	-	4,4,4	0.42	0	6,6,6	0.55	0
5	SO4	B	402	-	4,4,4	0.34	0	6,6,6	0.69	0
3	EDO	D	1002	-	3,3,3	0.34	0	2,2,2	0.87	0
5	SO4	A	401	-	4,4,4	0.17	0	6,6,6	0.57	0
5	SO4	A	406	-	4,4,4	0.35	0	6,6,6	0.95	0
3	EDO	D	1003	-	3,3,3	0.31	0	2,2,2	0.75	0
3	EDO	B	1002	-	3,3,3	0.38	0	2,2,2	0.51	0
5	SO4	C	407	-	4,4,4	0.27	0	6,6,6	0.40	0
5	SO4	C	404	-	4,4,4	0.40	0	6,6,6	0.40	0
3	EDO	D	1001	-	3,3,3	0.34	0	2,2,2	0.46	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	GOL	D	3002	-	-	2/4/4/4	-
3	EDO	A	1003	-	-	1/1/1/1	-
4	GOL	A	3002	-	-	2/4/4/4	-
3	EDO	C	2001	-	-	1/1/1/1	-
3	EDO	A	1001	-	-	1/1/1/1	-
3	EDO	D	1002	-	-	1/1/1/1	-
3	EDO	D	1003	-	-	1/1/1/1	-
3	EDO	B	1002	-	-	1/1/1/1	-
3	EDO	D	1001	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	3002	GOL	O1-C1-C2-O2
4	D	3002	GOL	O1-C1-C2-C3
4	A	3002	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	3002	GOL	O1-C1-C2-O2
3	A	1003	EDO	O1-C1-C2-O2
3	B	1002	EDO	O1-C1-C2-O2
3	C	2001	EDO	O1-C1-C2-O2
3	D	1002	EDO	O1-C1-C2-O2
3	D	1003	EDO	O1-C1-C2-O2
3	A	1001	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2001	EDO	1	0
5	A	406	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	261/272 (95%)	-0.10	3 (1%) 78 77	10, 17, 25, 41	0
1	B	260/272 (95%)	-0.06	5 (1%) 66 66	8, 19, 28, 53	2 (0%)
1	C	260/272 (95%)	-0.15	4 (1%) 72 71	8, 18, 28, 33	0
2	D	260/272 (95%)	-0.03	6 (2%) 61 60	13, 21, 28, 36	1 (0%)
All	All	1041/1088 (95%)	-0.09	18 (1%) 69 68	8, 19, 28, 53	3 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	SER	5.5
1	B	140	ASP	3.6
1	B	44	VAL	3.6
1	C	43	ASN	3.3
2	D	42	SER	3.1
1	C	42	SER	3.0
2	D	266	ASN	2.6
1	B	2	LYS	2.5
1	C	44	VAL	2.5
1	B	202	ILE	2.5
2	D	137	LEU	2.3
2	D	126	SER	2.3
1	A	7	ARG	2.3
1	C	137	LEU	2.2
1	A	42	SER	2.2
2	D	201	ASN	2.2
2	D	230	HIS	2.1
1	B	229	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSO	A	35	7/8	0.92	0.08	16,18,25,25	0
1	CSO	C	35	7/8	0.92	0.08	13,14,22,22	0
1	CSO	B	35	7/8	0.95	0.07	11,12,18,23	0

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
3	EDO	D	1002	4/4	0.71	0.23	54,54,55,57	0
3	EDO	A	1003	4/4	0.75	0.21	60,62,63,63	0
3	EDO	D	1003	4/4	0.75	0.28	60,60,60,61	0
3	EDO	B	1002	4/4	0.78	0.22	51,51,51,52	0
4	GOL	D	3002	6/6	0.80	0.16	55,59,61,64	0
3	EDO	C	2001	4/4	0.81	0.20	37,37,42,42	0
4	GOL	A	3002	6/6	0.82	0.17	48,51,54,55	0
5	SO4	C	407	5/5	0.83	0.09	76,76,77,77	0
5	SO4	C	405	5/5	0.86	0.11	72,73,74,75	0
3	EDO	D	1001	4/4	0.87	0.24	63,63,63,64	0
6	CL	C	601	1/1	0.90	0.20	66,66,66,66	0
6	CL	A	601	1/1	0.91	0.16	62,62,62,62	0
3	EDO	A	1001	4/4	0.91	0.20	45,46,47,48	0
5	SO4	A	406	5/5	0.93	0.27	46,47,53,59	0
5	SO4	D	403	5/5	0.93	0.12	41,44,47,50	0
5	SO4	C	404	5/5	0.95	0.14	49,50,53,53	0
5	SO4	A	401	5/5	0.96	0.10	32,38,40,40	0
5	SO4	B	402	5/5	0.96	0.09	41,43,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.