



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:17 AM UTC

PDB ID : 3OCE / pdb_00003oce
Title : Crystal structure of fumarate lyase:delta crystallin from Brucella melitensis bound to cobalt
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2010-08-09
Resolution : 2.58 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

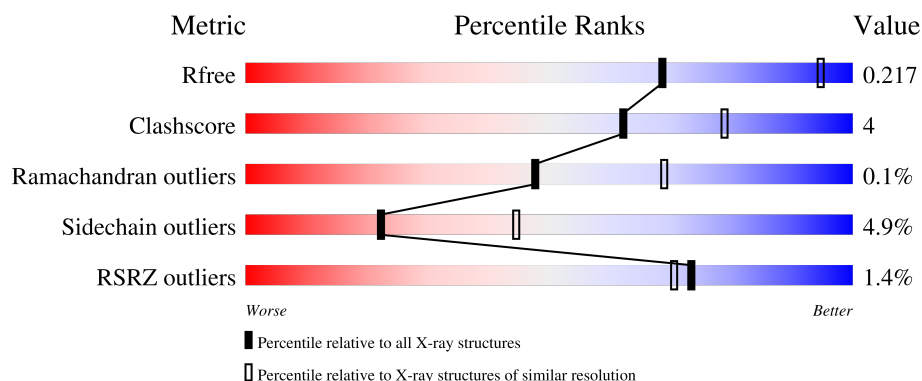
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	474	0% 87% 9% ..
1	B	474	86% 10% ..
1	C	474	3% 82% 13% ..
1	D	474	2% 85% 11% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14371 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 Fumarate lyase:Delta crystallin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	1	0
			3461	2169	613	663	16			
1	B	461	Total	C	N	O	S	0	0	0
			3451	2164	608	663	16			
1	C	460	Total	C	N	O	S	0	1	0
			3433	2153	607	657	16			
1	D	460	Total	C	N	O	S	0	2	0
			3462	2166	617	663	16			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q2YWLW1
A	-2	PRO	-	expression tag	UNP Q2YWLW1
A	-1	GLY	-	expression tag	UNP Q2YWLW1
A	0	SER	-	expression tag	UNP Q2YWLW1
A	1	MET	-	expression tag	UNP Q2YWLW1
B	-3	GLY	-	expression tag	UNP Q2YWLW1
B	-2	PRO	-	expression tag	UNP Q2YWLW1
B	-1	GLY	-	expression tag	UNP Q2YWLW1
B	0	SER	-	expression tag	UNP Q2YWLW1
B	1	MET	-	expression tag	UNP Q2YWLW1
C	-3	GLY	-	expression tag	UNP Q2YWLW1
C	-2	PRO	-	expression tag	UNP Q2YWLW1
C	-1	GLY	-	expression tag	UNP Q2YWLW1
C	0	SER	-	expression tag	UNP Q2YWLW1
C	1	MET	-	expression tag	UNP Q2YWLW1
D	-3	GLY	-	expression tag	UNP Q2YWLW1
D	-2	PRO	-	expression tag	UNP Q2YWLW1
D	-1	GLY	-	expression tag	UNP Q2YWLW1
D	0	SER	-	expression tag	UNP Q2YWLW1
D	1	MET	-	expression tag	UNP Q2YWLW1

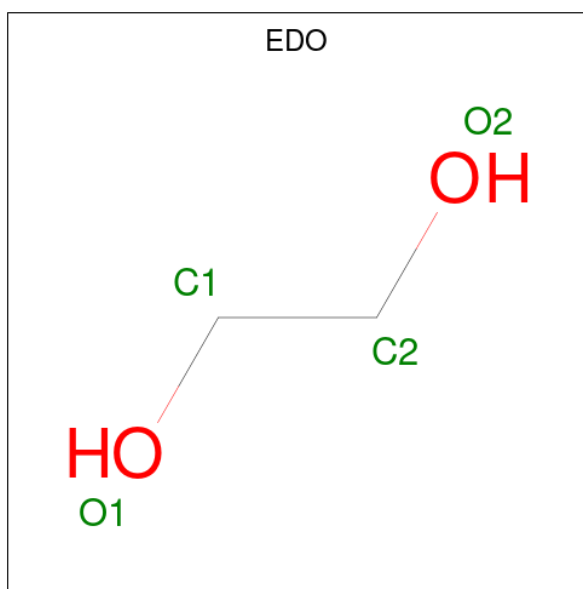
- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Co	0	0
			3	3		
2	B	3	Total	Co	0	0
			3	3		
2	C	3	Total	Co	0	0
			3	3		
2	D	3	Total	Co	0	0
			3	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

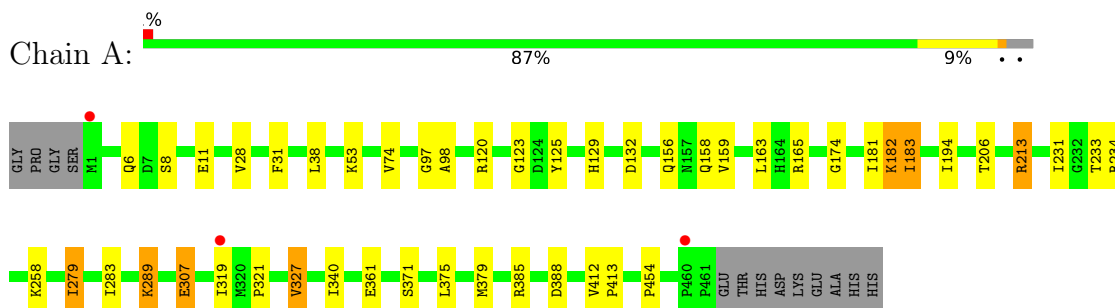
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	152	Total 152	O 152	0	0
5	B	135	Total 135	O 135	0	0
5	C	125	Total 125	O 125	0	0
5	D	132	Total 132	O 132	0	0

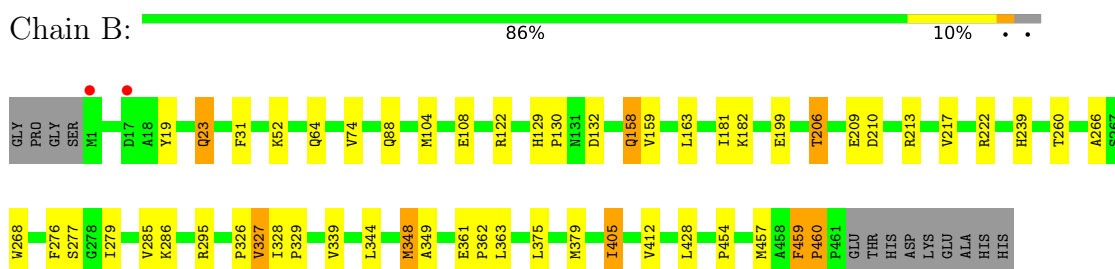
3 Residue-property plots [i](#)

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.

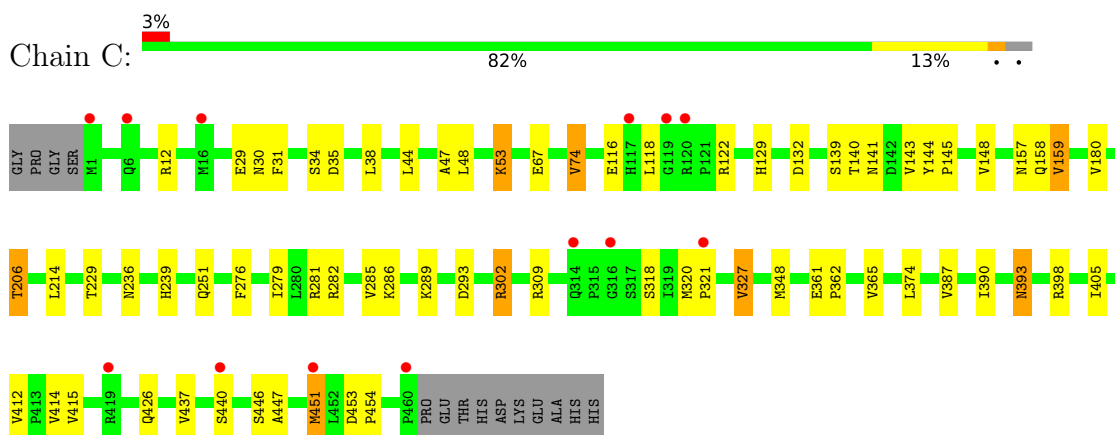
- Molecule 1: Fumarate lyase:Delta crystallin



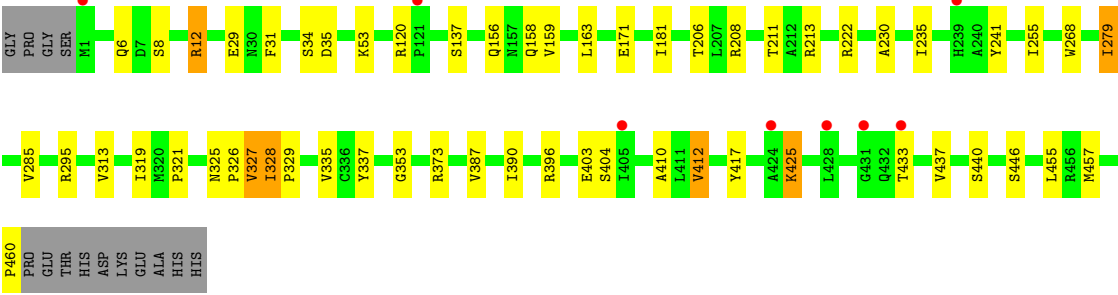
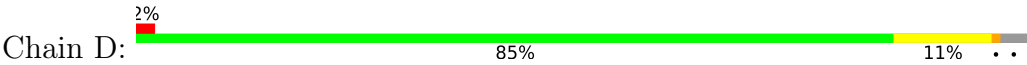
- Molecule 1: Fumarate lyase:Delta crystallin



- Molecule 1: Fumarate lyase:Delta crystallin



- Molecule 1: Fumarate lyase:Delta crystallin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.33Å 113.55Å 236.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.58 50.00 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.58) 98.8 (50.00-2.58)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.245 (Not available) , 0.217	Depositor DCC
R_{free} test set	4054 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14371	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5396e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CO, CL, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.89	2/3511 (0.1%)	1.07	5/4769 (0.1%)
1	B	0.86	2/3498 (0.1%)	1.05	4/4752 (0.1%)
1	C	0.88	0/3482	1.06	6/4732 (0.1%)
1	D	0.88	2/3514 (0.1%)	1.07	5/4770 (0.1%)
All	All	0.88	6/14005 (0.0%)	1.07	20/19023 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	412	VAL	CA-CB	7.63	1.57	1.54
1	D	279	ILE	CA-CB	5.74	1.62	1.54
1	B	460	PRO	CA-C	5.23	1.55	1.52
1	D	412	VAL	CA-CB	5.10	1.57	1.54
1	A	183	ILE	CA-CB	5.07	1.60	1.54
1	A	28	VAL	CA-CB	5.00	1.60	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	412	VAL	CA-C-N	-6.96	112.52	120.04
1	C	412	VAL	C-N-CA	-6.96	112.52	120.04
1	C	229	THR	N-CA-C	6.81	118.66	108.31
1	D	404	SER	N-CA-C	6.17	119.42	110.42
1	B	459	PHE	CA-C-N	5.66	123.74	119.66
1	B	459	PHE	C-N-CA	5.66	123.74	119.66
1	C	374	LEU	N-CA-C	5.60	117.83	111.11
1	D	353	GLY	N-CA-C	-5.60	104.92	112.14
1	C	141	ASN	N-CA-C	5.59	119.20	112.38
1	D	230	ALA	N-CA-C	5.40	117.59	111.11
1	B	210	ASP	N-CA-C	5.36	116.81	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ARG	CA-C-N	-5.31	114.87	120.66
1	A	120	ARG	C-N-CA	-5.31	114.87	120.66
1	A	361	GLU	CA-C-N	-5.24	113.24	119.05
1	A	361	GLU	C-N-CA	-5.24	113.24	119.05
1	C	30	ASN	N-CA-C	5.18	117.01	111.36
1	D	325	ASN	CA-C-N	5.13	126.25	119.84
1	D	325	ASN	C-N-CA	5.13	126.25	119.84
1	A	340	ILE	N-CA-C	5.09	115.82	110.62
1	B	209	GLU	N-CA-C	-5.05	105.85	111.36

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	3461	0	3510	29	0
1	B	3451	0	3497	36	0
1	C	3433	0	3469	39	0
1	D	3462	0	3507	33	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	6	1	0
5	A	152	0	0	1	0
5	B	135	0	0	3	0
5	C	125	0	0	1	0
5	D	132	0	0	2	0
All	All	14371	0	13989	114	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 4.

All (114) 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:B:327:VAL:HG13	1:D:31:PHE:CZ	2.11	0.85
1:B:327:VAL:HG13	1:D:31:PHE:HZ	1.40	0.85
1:B:31:PHE:CZ	1:D:327:VAL:HG13	2.14	0.83
1:D:171:GLU:OE2	1:D:208:ARG:NH1	2.13	0.81
1:B:31:PHE:HZ	1:D:327:VAL:HG13	1.48	0.77
1:D:437:VAL:O	1:D:440:SER:HB3	1.89	0.73
1:B:182:LYS:HE2	1:B:199:GLU:OE1	1.89	0.73
1:B:327:VAL:CG1	1:D:31:PHE:HZ	2.02	0.73
1:A:327:VAL:HG13	1:C:31:PHE:CE1	2.26	0.71
1:C:387:VAL:HA	1:C:390:ILE:HD12	1.73	0.68
1:C:279:ILE:HD12	1:C:282:ARG:HD3	1.78	0.64
1:A:327:VAL:HG13	1:C:31:PHE:HE1	1.62	0.63
1:B:182:LYS:CE	1:B:199:GLU:OE1	2.47	0.63
1:B:327:VAL:CG1	1:D:31:PHE:CZ	2.81	0.62
1:B:268:TRP:CE3	1:C:289:LYS:HE3	2.34	0.62
1:B:181:ILE:HG12	1:B:454:PRO:HB2	1.82	0.62
1:D:313:VAL:HG21	1:D:328:ILE:HD13	1.82	0.61
1:C:116:GLU:C	1:C:118:LEU:H	2.11	0.58
1:A:181:ILE:HG12	1:A:454:PRO:HB2	1.85	0.56
1:A:321:PRO:HD2	1:B:405:ILE:HG21	1.87	0.56
1:A:6:GLN:HG3	1:A:11:GLU:HG2	1.87	0.55
1:B:31:PHE:HZ	1:D:327:VAL:CG1	2.20	0.55
1:A:412:VAL:HB	1:A:413:PRO:HD3	1.90	0.54
1:D:12:ARG:NH2	1:D:29:GLU:OE1	2.41	0.54
1:D:410:ALA:HB2	1:D:457:MET:HE3	1.91	0.53
1:D:387:VAL:HA	1:D:390:ILE:HD12	1.91	0.53
1:D:412:VAL:HG22	1:D:417:TYR:HA	1.91	0.53
1:A:279:ILE:O	1:A:283:ILE:HG13	2.09	0.52
1:C:206:THR:OG1	1:C:286:LYS:CE	2.58	0.52
1:B:213:ARG:NH2	5:B:512:HOH:O	2.16	0.52
1:D:295:ARG:HG2	1:D:326:PRO:HB2	1.92	0.52
1:B:23:GLN:HB2	1:B:108:GLU:OE2	2.10	0.52
1:A:289:LYS:HE2	1:D:268:TRP:CE3	2.45	0.51
1:C:321:PRO:HG3	1:D:425:LYS:HA	1.93	0.51
1:A:53:LYS:NZ	5:A:594:HOH:O	2.42	0.50
1:B:260:THR:HG21	1:B:266:ALA:CB	2.41	0.50
1:C:236:ASN:HB3	5:C:573:HOH:O	2.11	0.50
1:C:276:PHE:O	1:C:279:ILE:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:VAL:HG12	1:C:415:VAL:HG13	1.94	0.50
1:D:208:ARG:HD3	5:D:497:HOH:O	2.11	0.49
1:D:213[A]:ARG:NH2	5:D:546:HOH:O	2.38	0.49
1:A:233:THR:O	1:A:234:ARG:HB2	2.13	0.49
1:C:447:ALA:O	1:C:451:MET:HB2	2.11	0.49
1:C:302:ARG:HG2	1:D:403:GLU:CG	2.43	0.49
1:C:302:ARG:HG2	1:D:403:GLU:HG2	1.94	0.49
1:C:387:VAL:HA	1:C:390:ILE:CD1	2.42	0.49
1:A:31:PHE:CE1	1:C:327:VAL:HG13	2.48	0.48
1:A:129:HIS:HB3	1:A:132:ASP:HB2	1.94	0.48
1:A:182:LYS:HE2	1:A:307:GLU:OE1	2.13	0.48
1:A:31:PHE:CZ	1:C:327:VAL:HG13	2.49	0.48
1:C:281:ARG:O	1:C:285:VAL:HG23	2.13	0.48
1:A:327:VAL:HG13	1:C:31:PHE:CZ	2.49	0.47
1:D:241:TYR:CD2	1:D:241:TYR:C	2.93	0.47
1:B:260:THR:HG21	1:B:266:ALA:HB2	1.97	0.47
1:C:129:HIS:HB3	1:C:132:ASP:HB2	1.96	0.47
1:A:321:PRO:HB2	1:B:428:LEU:HD22	1.97	0.47
1:D:12:ARG:HH22	1:D:29:GLU:CD	2.23	0.47
1:B:158:GLN:HG3	5:B:609:HOH:O	2.16	0.47
1:A:174:GLY:O	4:A:475:EDO:H21	2.15	0.46
1:B:31:PHE:CE1	1:D:327:VAL:HG13	2.50	0.46
1:B:348:MET:HE2	1:D:337:TYR:CD1	2.51	0.46
1:D:222:ARG:NH1	1:D:255:ILE:HG23	2.30	0.46
1:A:183:ILE:HD12	1:A:183:ILE:HA	1.80	0.46
1:B:295:ARG:HG2	1:B:326:PRO:HB2	1.97	0.46
1:C:405:ILE:HG21	1:D:321:PRO:HD2	1.98	0.46
1:A:182:LYS:HG3	1:A:194:ILE:O	2.16	0.46
1:A:97:GLY:O	1:A:98:ALA:HB3	2.16	0.46
1:C:309:ARG:NH1	1:C:393:ASN:OD1	2.49	0.46
1:C:139:SER:O	1:C:140:THR:C	2.59	0.46
1:C:116:GLU:C	1:C:118:LEU:N	2.69	0.45
1:A:319:ILE:C	1:A:321:PRO:HD3	2.42	0.45
1:C:289:LYS:NZ	1:C:293:ASP:OD1	2.49	0.45
1:D:34:SER:O	1:D:35:ASP:HB2	2.15	0.45
1:A:53:LYS:HE3	1:A:74:VAL:HG13	1.97	0.44
1:B:361:GLU:N	1:B:362:PRO:CD	2.80	0.44
1:B:328:ILE:HB	1:B:329:PRO:HD3	2.00	0.44
1:C:12:ARG:NH2	1:C:29:GLU:OE2	2.49	0.44
1:B:163:LEU:HG	1:B:379:MET:HE1	2.00	0.43
1:C:348:MET:HE3	1:C:348:MET:HB3	1.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:VAL:HG21	1:B:375:LEU:HG	2.00	0.43
1:C:148:VAL:HG13	1:C:365:VAL:HG23	2.00	0.43
1:B:344:LEU:HD12	1:B:344:LEU:O	2.18	0.43
1:B:129:HIS:HB3	1:B:132:ASP:HB2	1.99	0.43
1:A:234:ARG:HD2	1:D:460:PRO:HG3	2.01	0.43
1:C:437:VAL:O	1:C:440:SER:HB2	2.18	0.43
1:C:159:VAL:HG22	1:C:214:LEU:CD2	2.49	0.42
1:B:349:ALA:HB2	1:B:363:LEU:HD23	2.01	0.42
1:B:454:PRO:HA	1:B:457:MET:HG3	2.00	0.42
1:A:165:ARG:NH2	1:A:388:ASP:OD2	2.44	0.42
1:C:38:LEU:HD11	1:C:44:LEU:HD23	2.02	0.42
1:C:53:LYS:HG3	1:C:74:VAL:HG22	2.01	0.42
1:B:206:THR:OG1	1:B:286:LYS:HE3	2.19	0.42
1:C:453:ASP:HA	1:C:454:PRO:HD3	1.94	0.42
1:B:459:PHE:HA	1:B:460:PRO:HD2	1.84	0.42
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.97	0.41
1:B:217:VAL:HG12	1:B:276:PHE:HD1	1.83	0.41
1:A:213:ARG:HD3	1:A:213:ARG:HA	1.85	0.41
1:B:19:TYR:HB2	1:B:88:GLN:HG3	2.02	0.41
1:C:148:VAL:HG13	1:C:365:VAL:CG2	2.51	0.41
1:C:159:VAL:HG22	1:C:214:LEU:HD21	2.02	0.41
1:D:328:ILE:O	1:D:329:PRO:C	2.64	0.41
1:B:239:HIS:HE1	5:B:576:HOH:O	2.04	0.41
1:C:34:SER:O	1:C:35:ASP:HB2	2.20	0.41
1:A:123:GLY:HA2	1:A:125:TYR:CZ	2.57	0.40
1:A:231:ILE:HG13	1:A:233:THR:HG23	2.03	0.40
1:A:163:LEU:HG	1:A:379:MET:HE1	2.04	0.40
1:B:23:GLN:OE1	1:B:104:MET:HE2	2.21	0.40
1:C:47:ALA:O	1:C:48:LEU:C	2.65	0.40
1:D:156:GLN:OE1	1:D:156:GLN:HA	2.19	0.40
1:D:163:LEU:HD13	1:D:211:THR:HG22	2.03	0.40
1:D:181:ILE:HD13	1:D:455:LEU:HA	2.03	0.40
1:B:129:HIS:HA	1:B:130:PRO:HD3	1.93	0.40
1:C:144:TYR:N	1:C:145:PRO:HD2	2.36	0.40
1:C:361:GLU:N	1:C:362:PRO:CD	2.85	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	460/474 (97%)	447 (97%)	12 (3%)	1 (0%)	43	63
1	B	459/474 (97%)	449 (98%)	10 (2%)	0	100	100
1	C	459/474 (97%)	443 (96%)	15 (3%)	1 (0%)	43	63
1	D	460/474 (97%)	450 (98%)	10 (2%)	0	100	100
All	All	1838/1896 (97%)	1789 (97%)	47 (3%)	2 (0%)	48	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	C	180	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	363/377 (96%)	349 (96%)	14 (4%)	28	53
1	B	362/377 (96%)	347 (96%)	15 (4%)	27	51
1	C	357/377 (95%)	337 (94%)	20 (6%)	19	38
1	D	362/377 (96%)	341 (94%)	21 (6%)	18	37
All	All	1444/1508 (96%)	1374 (95%)	70 (5%)	22	45

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	156	GLN
1	A	158	GLN
1	A	159	VAL
1	A	182	LYS
1	A	206	THR
1	A	213	ARG
1	A	258	LYS
1	A	279	ILE
1	A	289	LYS
1	A	307	GLU
1	A	327	VAL
1	A	371	SER
1	A	385	ARG
1	B	23	GLN
1	B	52	LYS
1	B	64	GLN
1	B	74	VAL
1	B	122	ARG
1	B	158	GLN
1	B	159	VAL
1	B	206	THR
1	B	222	ARG
1	B	277	SER
1	B	279	ILE
1	B	285	VAL
1	B	327	VAL
1	B	348	MET
1	B	405	ILE
1	C	53	LYS
1	C	67	GLU
1	C	74	VAL
1	C	122	ARG
1	C	143	VAL
1	C	157	ASN
1	C	158	GLN
1	C	159	VAL
1	C	206	THR
1	C	239	HIS
1	C	251	GLN
1	C	302	ARG
1	C	318	SER
1	C	320	MET

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Mol	Chain	Res	Type
1	C	327	VAL
1	C	393	ASN
1	C	398	ARG
1	C	426	GLN
1	C	446	SER
1	C	451	MET
1	D	6	GLN
1	D	8	SER
1	D	12	ARG
1	D	53	LYS
1	D	120	ARG
1	D	137	SER
1	D	158	GLN
1	D	159	VAL
1	D	206	THR
1	D	235	ILE
1	D	279	ILE
1	D	285	VAL
1	D	319	ILE
1	D	327	VAL
1	D	328	ILE
1	D	335	VAL
1	D	373	ARG
1	D	396	ARG
1	D	425	LYS
1	D	433	THR
1	D	446	SER

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

Mol	Chain	Res	Type
1	A	39	ASN
1	A	157	ASN
1	A	187	GLN
1	A	251	GLN
1	B	59	ASN
1	B	432	GLN
1	C	117	HIS
1	C	131	ASN
1	C	156	GLN
1	C	236	ASN
1	C	334	GLN

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Mol	Chain	Res	Type
1	D	225	ASN
1	D	426	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 16 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	A	475	-	3,3,3	0.56	0	2,2,2	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	475	-	-	1/1/1/1	-

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
4	A	475	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	475	EDO	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	461/474 (97%)	-0.31	3 (0%) 84 82	12, 24, 49, 67	1 (0%)
1	B	461/474 (97%)	-0.29	2 (0%) 88 87	12, 26, 49, 69	0
1	C	460/474 (97%)	-0.05	13 (2%) 55 50	12, 29, 57, 74	1 (0%)
1	D	460/474 (97%)	-0.10	8 (1%) 69 65	13, 29, 63, 74	2 (0%)
All	All	1842/1896 (97%)	-0.19	26 (1%) 73 70	12, 27, 55, 74	4 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	4.7
1	A	1	MET	3.7
1	B	1	MET	3.3
1	C	460	PRO	3.3
1	C	119	GLY	3.2
1	A	319	ILE	3.1
1	C	1	MET	3.1
1	C	440	SER	2.9
1	C	419	ARG	2.7
1	D	431	GLY	2.5
1	D	405	ILE	2.3
1	C	117	HIS	2.3
1	D	428	LEU	2.2
1	D	424	ALA	2.2
1	C	6	GLN	2.2
1	A	460	PRO	2.2
1	C	451	MET	2.1
1	D	121	PRO	2.1
1	C	316	GLY	2.1
1	C	120	ARG	2.1
1	B	17	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	321	PRO	2.1
1	C	314	GLN	2.0
1	C	16	MET	2.0
1	D	433	THR	2.0
1	D	239	HIS	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 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
2	CO	B	473	1/1	0.87	0.07	54,54,54,54	0
4	EDO	A	475	4/4	0.87	0.12	27,30,31,35	0
2	CO	C	473	1/1	0.92	0.05	44,44,44,44	0
2	CO	A	473	1/1	0.93	0.06	56,56,56,56	0
2	CO	D	473	1/1	0.94	0.06	50,50,50,50	0
3	CL	D	474	1/1	0.95	0.09	27,27,27,27	0
3	CL	A	474	1/1	0.96	0.10	42,42,42,42	0
2	CO	A	472	1/1	0.97	0.05	38,38,38,38	0
2	CO	B	472	1/1	0.98	0.08	33,33,33,33	0
3	CL	C	474	1/1	0.98	0.08	23,23,23,23	0
3	CL	B	474	1/1	0.99	0.08	23,23,23,23	0
2	CO	D	472	1/1	0.99	0.06	27,27,27,27	0
2	CO	C	472	1/1	0.99	0.03	33,33,33,33	0
2	CO	D	471	1/1	0.99	0.04	8,8,8,8	0
2	CO	B	471	1/1	1.00	0.08	9,9,9,9	0
2	CO	C	471	1/1	1.00	0.05	14,14,14,14	0
2	CO	A	471	1/1	1.00	0.05	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.