



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:22 am GMT

PDB ID : 3OCF
Title : Crystal structure of fumarate lyase:delta crystallin from Brucella melitensis in native form
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2010-08-09
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

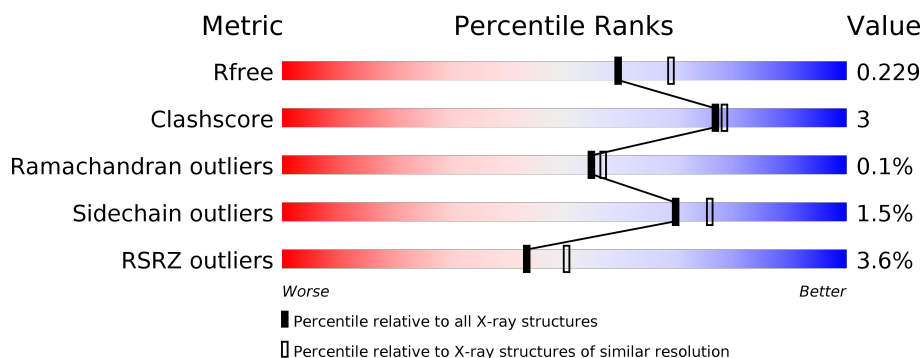
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	478	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>7%</div> </div> </div>
1	B	478	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>6%</div> <div>10%</div> </div> </div>
1	C	478	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>
1	D	478	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>10%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	460	-	-	-	X
3	EDO	B	459	-	-	-	X
3	EDO	D	459	-	-	-	X
3	EDO	D	460	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13594 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	444	Total	C	N	O	S	0	2	0
			3278	2058	582	625	13			
1	B	430	Total	C	N	O	S	0	3	0
			3167	1987	561	605	14			
1	C	444	Total	C	N	O	S	0	5	0
			3303	2074	579	636	14			
1	D	430	Total	C	N	O	S	0	3	0
			3189	1994	565	617	13			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q2YWLW1
A	-19	ALA	-	EXPRESSION TAG	UNP Q2YWLW1
A	-18	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
A	-17	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
A	-16	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
A	-15	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
A	-14	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
A	-13	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
A	-12	MET	-	EXPRESSION TAG	UNP Q2YWLW1
A	-11	GLY	-	EXPRESSION TAG	UNP Q2YWLW1
A	-10	THR	-	EXPRESSION TAG	UNP Q2YWLW1
A	-9	LEU	-	EXPRESSION TAG	UNP Q2YWLW1
A	-8	GLU	-	EXPRESSION TAG	UNP Q2YWLW1
A	-7	ALA	-	EXPRESSION TAG	UNP Q2YWLW1
A	-6	GLN	-	EXPRESSION TAG	UNP Q2YWLW1
A	-5	THR	-	EXPRESSION TAG	UNP Q2YWLW1
A	-4	GLN	-	EXPRESSION TAG	UNP Q2YWLW1
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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q2YWLW1
B	-20	MET	-	EXPRESSION TAG	UNP Q2YWLW1
B	-19	ALA	-	EXPRESSION TAG	UNP Q2YWLW1
B	-18	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
B	-17	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
B	-16	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
B	-15	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
B	-14	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
B	-13	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
B	-12	MET	-	EXPRESSION TAG	UNP Q2YWLW1
B	-11	GLY	-	EXPRESSION TAG	UNP Q2YWLW1
B	-10	THR	-	EXPRESSION TAG	UNP Q2YWLW1
B	-9	LEU	-	EXPRESSION TAG	UNP Q2YWLW1
B	-8	GLU	-	EXPRESSION TAG	UNP Q2YWLW1
B	-7	ALA	-	EXPRESSION TAG	UNP Q2YWLW1
B	-6	GLN	-	EXPRESSION TAG	UNP Q2YWLW1
B	-5	THR	-	EXPRESSION TAG	UNP Q2YWLW1
B	-4	GLN	-	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	-20	MET	-	EXPRESSION TAG	UNP Q2YWLW1
C	-19	ALA	-	EXPRESSION TAG	UNP Q2YWLW1
C	-18	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
C	-17	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
C	-16	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
C	-15	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
C	-14	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
C	-13	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
C	-12	MET	-	EXPRESSION TAG	UNP Q2YWLW1
C	-11	GLY	-	EXPRESSION TAG	UNP Q2YWLW1
C	-10	THR	-	EXPRESSION TAG	UNP Q2YWLW1
C	-9	LEU	-	EXPRESSION TAG	UNP Q2YWLW1
C	-8	GLU	-	EXPRESSION TAG	UNP Q2YWLW1
C	-7	ALA	-	EXPRESSION TAG	UNP Q2YWLW1
C	-6	GLN	-	EXPRESSION TAG	UNP Q2YWLW1
C	-5	THR	-	EXPRESSION TAG	UNP Q2YWLW1
C	-4	GLN	-	EXPRESSION TAG	UNP Q2YWLW1
C	-3	GLY	-	EXPRESSION TAG	UNP Q2YWLW1
C	-2	PRO	-	EXPRESSION TAG	UNP Q2YWLW1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP Q2YWLW1
C	0	SER	-	EXPRESSION TAG	UNP Q2YWLW1
C	1	MET	-	EXPRESSION TAG	UNP Q2YWLW1
D	-20	MET	-	EXPRESSION TAG	UNP Q2YWLW1
D	-19	ALA	-	EXPRESSION TAG	UNP Q2YWLW1
D	-18	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
D	-17	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
D	-16	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
D	-15	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
D	-14	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
D	-13	HIS	-	EXPRESSION TAG	UNP Q2YWLW1
D	-12	MET	-	EXPRESSION TAG	UNP Q2YWLW1
D	-11	GLY	-	EXPRESSION TAG	UNP Q2YWLW1
D	-10	THR	-	EXPRESSION TAG	UNP Q2YWLW1
D	-9	LEU	-	EXPRESSION TAG	UNP Q2YWLW1
D	-8	GLU	-	EXPRESSION TAG	UNP Q2YWLW1
D	-7	ALA	-	EXPRESSION TAG	UNP Q2YWLW1
D	-6	GLN	-	EXPRESSION TAG	UNP Q2YWLW1
D	-5	THR	-	EXPRESSION TAG	UNP Q2YWLW1
D	-4	GLN	-	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

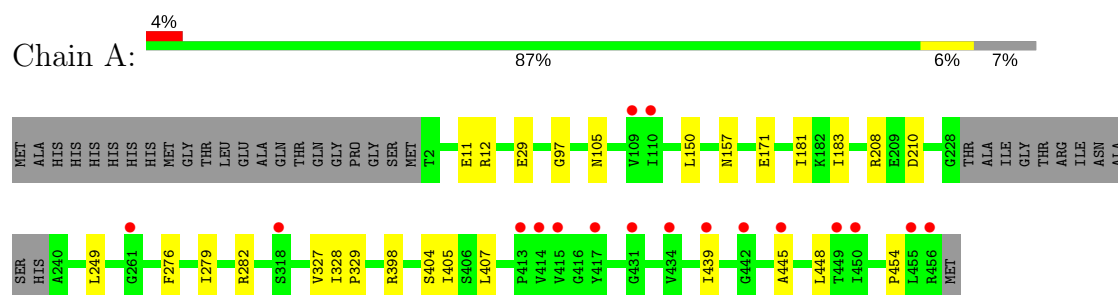
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	167	Total	O	0	0
			167	167		
4	B	127	Total	O	0	0
			127	127		
4	C	146	Total	O	0	0
			146	146		
4	D	193	Total	O	0	0
			193	193		

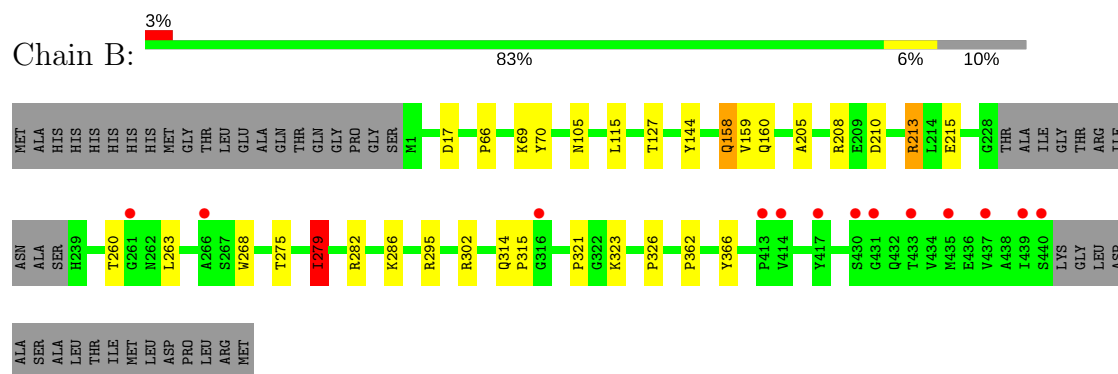
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

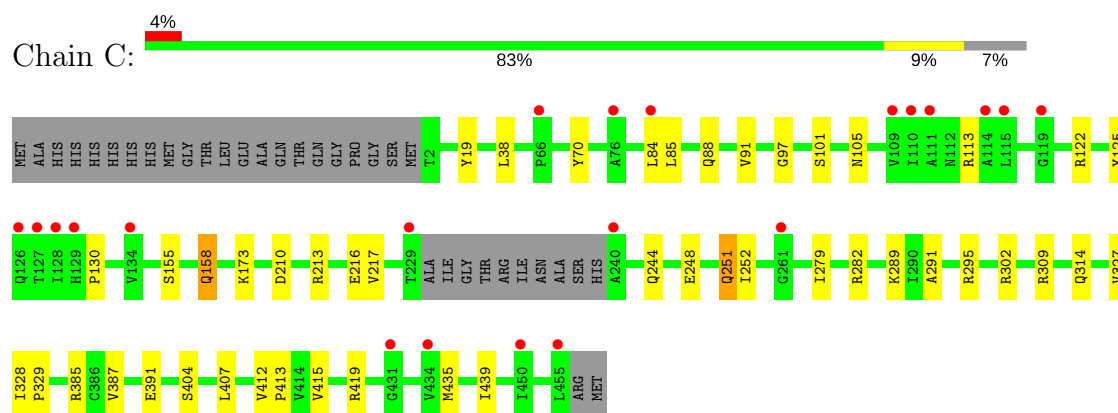
• Molecule 1: Fumarate lyase:Delta crystallin



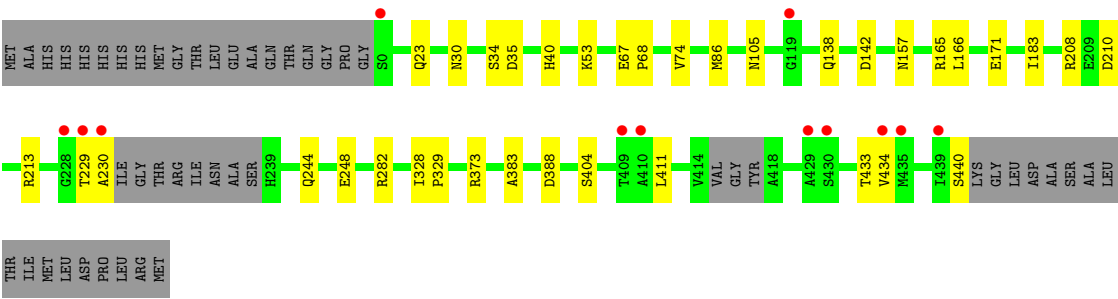
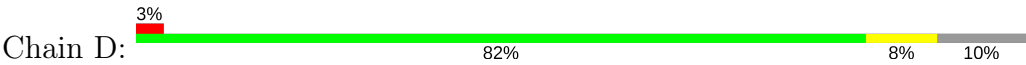
• Molecule 1: Fumarate lyase:Delta crystallin



• Molecule 1: Fumarate lyase:Delta crystallin



• Molecule 1: Fumarate lyase:Delta crystallin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.23Å 86.46Å 105.16Å 90.00° 91.91° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 19.73 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.10) 99.5 (19.73-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.171 , 0.227 0.176 , 0.229	Depositor DCC
R_{free} test set	4501 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l 0.013 for k,h,-l 0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13594	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: 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	0.72	0/3327	0.70	0/4525
1	B	0.71	0/3218	0.69	1/4379 (0.0%)
1	C	0.69	0/3361	0.70	1/4574 (0.0%)
1	D	0.75	0/3238	0.74	0/4401
All	All	0.72	0/13144	0.71	2/17879 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	LEU	CA-CB-CG	7.53	132.62	115.30
1	B	279	ILE	CG1-CB-CG2	-5.16	100.06	111.40

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	3278	0	3280	19	0
1	B	3167	0	3149	25	0
1	C	3303	0	3307	29	0
1	D	3189	0	3174	24	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	12	1	0
3	B	4	0	6	1	0
3	D	8	0	12	0	0
4	A	167	0	0	3	0
4	B	127	0	0	5	0
4	C	146	0	0	2	0
4	D	193	0	0	3	0
All	All	13594	0	12940	90	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 3.

All (90) 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:208:ARG:NH1	4:B:517:HOH:O	2.17	0.76
4:A:548:HOH:O	1:C:314[B]:GLN:CG	2.34	0.75
1:A:181:ILE:HD11	1:A:398[A]:ARG:HG3	1.68	0.74
1:A:183:ILE:HD13	1:A:404:SER:HB2	1.68	0.74
4:A:548:HOH:O	1:C:314[B]:GLN:HG3	1.90	0.71
1:D:229:THR:HG23	1:D:230:ALA:N	2.08	0.69
3:A:459:EDO:H22	3:A:460:EDO:H12	1.74	0.69
1:D:229:THR:HG23	1:D:230:ALA:H	1.59	0.66
1:A:405:ILE:HG21	1:B:321:PRO:HD2	1.78	0.64
1:C:309:ARG:NH1	1:C:391[A]:GLU:OE2	2.31	0.63
1:A:12:ARG:NH2	1:A:29:GLU:OE2	2.31	0.63
1:D:183:ILE:HD13	1:D:404:SER:HB2	1.80	0.63
1:D:67:GLU:N	1:D:68:PRO:HD2	2.16	0.60
1:C:314[B]:GLN:NE2	4:C:597:HOH:O	2.33	0.60
1:B:323:LYS:HE3	4:B:487:HOH:O	2.02	0.59
1:C:210:ASP:OD1	1:C:282[A]:ARG:NH2	2.37	0.56
1:D:53:LYS:HE3	1:D:74:VAL:HG13	1.87	0.56
1:B:366:TYR:CE2	3:B:459:EDO:H12	2.41	0.56
1:B:282:ARG:HD2	1:B:286:LYS:HE3	1.88	0.55
1:B:66:PRO:HD2	1:B:69:LYS:HE2	1.88	0.55
1:B:210:ASP:OD1	1:B:282:ARG:NH1	2.40	0.54
1:A:439:ILE:HD11	1:A:445:ALA:HB2	1.90	0.54
1:B:314:GLN:OE1	1:D:30:ASN:ND2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:VAL:HB	1:C:419:ARG:HD3	1.91	0.53
1:C:85:LEU:HD11	1:C:113:ARG:HD3	1.90	0.53
1:A:276:PHE:O	1:A:279:ILE:HG22	2.09	0.53
1:A:11:GLU:O	1:A:12:ARG:HD2	2.09	0.53
1:D:157:ASN:ND2	4:D:592:HOH:O	2.42	0.53
1:B:205:ALA:HA	1:B:208:ARG:NH1	2.25	0.52
1:D:138:GLN:HA	1:D:229:THR:HG21	1.91	0.52
1:A:407:LEU:HB3	1:A:448:LEU:HD22	1.91	0.52
1:D:244:GLN:O	1:D:248:GLU:HG2	2.11	0.50
1:C:173:LYS:HE3	1:C:387:VAL:O	2.12	0.50
1:B:268:TRP:CE3	1:C:289:LYS:HE3	2.47	0.49
1:A:208:ARG:HD3	4:A:566:HOH:O	2.10	0.49
1:B:213:ARG:HG2	1:B:279:ILE:HD13	1.94	0.49
1:B:275:THR:HG23	1:C:282[B]:ARG:NH2	2.27	0.49
1:D:328:ILE:HB	1:D:329:PRO:HD3	1.95	0.48
1:C:217:VAL:HG21	1:C:279:ILE:HD11	1.95	0.48
1:A:327:VAL:HG12	1:C:97:GLY:HA2	1.96	0.48
1:B:158:GLN:HG2	1:B:159:VAL:N	2.29	0.47
1:B:323:LYS:CE	4:B:487:HOH:O	2.62	0.47
1:D:229:THR:CG2	1:D:230:ALA:N	2.77	0.47
1:C:279:ILE:HG13	1:C:282[B]:ARG:NH2	2.29	0.47
1:D:373:ARG:NH1	4:D:622:HOH:O	2.45	0.47
1:C:19:TYR:HB2	1:C:88:GLN:HG3	1.95	0.47
1:A:150:LEU:HD22	1:A:249:LEU:HD11	1.97	0.47
1:A:97:GLY:HA2	1:C:327:VAL:HG12	1.96	0.47
1:C:435:MET:O	1:C:439:ILE:HG12	2.15	0.46
1:A:407:LEU:HB3	1:A:448:LEU:CD2	2.46	0.46
1:B:160:GLN:NE2	1:B:215:GLU:HG2	2.30	0.46
1:C:244:GLN:O	1:C:248:GLU:HG2	2.15	0.46
1:A:210:ASP:OD1	1:A:282:ARG:NE	2.49	0.46
1:D:229:THR:CG2	1:D:230:ALA:H	2.28	0.46
1:C:385:ARG:NH2	4:C:594:HOH:O	2.49	0.45
1:C:404:SER:HB3	1:C:407:LEU:HG	1.97	0.45
1:C:217:VAL:HG21	1:C:279:ILE:CD1	2.47	0.45
1:D:433:THR:HB	4:D:626:HOH:O	2.16	0.45
1:C:91:VAL:HG11	1:C:101:SER:HB3	1.99	0.45
1:B:115:LEU:HD21	1:B:127:THR:HB	1.99	0.44
1:B:213:ARG:HG2	1:B:282:ARG:NH2	2.33	0.44
1:D:165:ARG:NH2	1:D:388:ASP:OD2	2.41	0.44
1:C:125:TYR:CD1	1:C:130:PRO:HD3	2.52	0.43
1:D:142:ASP:OD2	1:D:229:THR:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:VAL:HB	1:C:413:PRO:HD3	2.01	0.43
1:D:434:VAL:HG12	1:D:434:VAL:O	2.19	0.43
1:D:166:LEU:HA	1:D:383:ALA:HB2	2.00	0.43
1:B:295:ARG:HG2	1:B:326:PRO:HB2	2.01	0.43
1:C:122:ARG:HG2	1:C:122:ARG:HH11	1.84	0.42
1:D:210:ASP:OD1	1:D:282:ARG:NH2	2.47	0.42
1:A:12:ARG:HH22	1:A:29:GLU:CD	2.20	0.42
1:A:150:LEU:CD2	1:A:249:LEU:HD11	2.50	0.42
1:D:171:GLU:HG2	1:D:208:ARG:HH11	1.84	0.42
1:B:315:PRO:HG2	1:D:23:GLN:NE2	2.34	0.42
1:C:213:ARG:HA	1:C:216:GLU:HG2	2.02	0.42
1:C:328:ILE:HB	1:C:329:PRO:HD3	2.02	0.42
1:A:171:GLU:OE2	1:A:208:ARG:NH1	2.50	0.42
1:B:144:TYR:OH	1:B:362:PRO:HA	2.20	0.42
1:A:181:ILE:HG23	1:A:454:PRO:HG3	2.01	0.41
1:B:315:PRO:HG3	1:D:23:GLN:HG2	2.02	0.41
1:C:291:ALA:O	1:C:295:ARG:HG3	2.20	0.41
1:B:158:GLN:HG3	4:B:491:HOH:O	2.19	0.41
1:D:67:GLU:N	1:D:68:PRO:CD	2.83	0.41
1:B:323:LYS:NZ	4:B:487:HOH:O	2.50	0.40
1:A:328:ILE:HB	1:A:329:PRO:HD3	2.02	0.40
1:B:260:THR:CG2	1:B:263:LEU:HD23	2.51	0.40
1:C:155:SER:O	1:C:158:GLN:HG3	2.21	0.40
1:D:34:SER:O	1:D:35:ASP:HB2	2.21	0.40
1:C:251:GLN:HG3	1:C:252:ILE:N	2.37	0.40
1:B:205:ALA:HA	1:B:208:ARG:HH12	1.86	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	442/478 (92%)	436 (99%)	6 (1%)	0	100	100
1	B	429/478 (90%)	415 (97%)	14 (3%)	0	100	100
1	C	445/478 (93%)	432 (97%)	12 (3%)	1 (0%)	51	52
1	D	427/478 (89%)	417 (98%)	10 (2%)	0	100	100
All	All	1743/1912 (91%)	1700 (98%)	42 (2%)	1 (0%)	55	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	70	TYR

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	334/380 (88%)	332 (99%)	2 (1%)	89	92
1	B	321/380 (84%)	314 (98%)	7 (2%)	57	62
1	C	341/380 (90%)	336 (98%)	5 (2%)	70	76
1	D	327/380 (86%)	320 (98%)	7 (2%)	59	64
All	All	1323/1520 (87%)	1302 (98%)	21 (2%)	70	74

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

Mol	Chain	Res	Type
1	A	105	ASN
1	A	157	ASN
1	B	17	ASP
1	B	70	TYR
1	B	105	ASN
1	B	158	GLN
1	B	213	ARG
1	B	279	ILE
1	B	302	ARG
1	C	84	LEU

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Mol	Chain	Res	Type
1	C	105	ASN
1	C	158	GLN
1	C	251	GLN
1	C	302	ARG
1	D	40[A]	HIS
1	D	40[B]	HIS
1	D	86	MET
1	D	105	ASN
1	D	213	ARG
1	D	411	LEU
1	D	440	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	158	GLN
1	B	160	GLN
1	D	23	GLN
1	D	131	ASN
1	D	157	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	EDO	A	459	-	3,3,3	0.26	0	2,2,2	0.77	0
3	EDO	A	460	-	3,3,3	0.41	0	2,2,2	1.05	0
3	EDO	B	459	-	3,3,3	0.28	0	2,2,2	0.37	0
3	EDO	D	459	-	3,3,3	0.59	0	2,2,2	0.46	0
3	EDO	D	460	-	3,3,3	0.38	0	2,2,2	1.29	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	EDO	A	459	-	-	0/1/1/1	0/0/0/0
3	EDO	A	460	-	-	0/1/1/1	0/0/0/0
3	EDO	B	459	-	-	0/1/1/1	0/0/0/0
3	EDO	D	459	-	-	0/1/1/1	0/0/0/0
3	EDO	D	460	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	459	EDO	1	0
3	A	460	EDO	1	0
3	B	459	EDO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/478 (92%)	-0.24	17 (3%) 41 48	16, 27, 56, 70	0
1	B	430/478 (89%)	-0.19	13 (3%) 51 58	16, 31, 57, 69	0
1	C	444/478 (92%)	-0.04	21 (4%) 32 38	17, 35, 62, 76	0
1	D	430/478 (89%)	-0.30	12 (2%) 53 60	16, 26, 57, 76	0
All	All	1748/1912 (91%)	-0.19	63 (3%) 43 50	16, 29, 59, 76	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	ALA	4.6
1	D	0	SER	4.5
1	A	413	PRO	3.9
1	A	414	VAL	3.9
1	C	229	THR	3.7
1	D	430	SER	3.7
1	B	414	VAL	3.7
1	B	430	SER	3.5
1	D	230	ALA	3.5
1	C	110	ILE	3.3
1	A	442	GLY	3.2
1	D	429	ALA	3.2
1	B	435	MET	3.2
1	C	126	GLN	3.2
1	B	316	GLY	3.1
1	A	431	GLY	3.1
1	A	415	VAL	3.1
1	A	261	GLY	3.1
1	B	417	TYR	3.1
1	C	455	LEU	3.0
1	B	439	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	109	VAL	3.0
1	D	229	THR	3.0
1	B	413	PRO	2.9
1	D	434	VAL	2.9
1	C	261	GLY	2.9
1	D	439	ILE	2.8
1	A	455	LEU	2.8
1	C	128	ILE	2.7
1	D	410	ALA	2.7
1	C	66	PRO	2.6
1	C	111	ALA	2.6
1	C	127	THR	2.6
1	B	261	GLY	2.6
1	A	449	THR	2.6
1	C	434	VAL	2.6
1	B	431	GLY	2.6
1	C	84	LEU	2.6
1	C	129	HIS	2.5
1	A	450	ILE	2.5
1	D	409	THR	2.5
1	A	434	VAL	2.4
1	A	456	ARG	2.4
1	B	440	SER	2.4
1	C	134	VAL	2.3
1	C	119	GLY	2.3
1	B	266	ALA	2.3
1	A	417	TYR	2.3
1	A	110	ILE	2.2
1	A	439	ILE	2.2
1	C	240	ALA	2.2
1	C	450	ILE	2.2
1	B	437	VAL	2.2
1	D	435	MET	2.2
1	A	318	SER	2.1
1	C	115	LEU	2.1
1	C	76	ALA	2.1
1	C	114	ALA	2.1
1	C	431	GLY	2.1
1	D	228	GLY	2.0
1	A	109	VAL	2.0
1	B	433	THR	2.0
1	D	119	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	EDO	D	460	4/4	0.88	0.17	7.44	23,26,31,34	0
3	EDO	A	460	4/4	0.95	0.12	2.83	19,21,25,30	0
3	EDO	B	459	4/4	0.95	0.10	2.22	22,27,31,35	0
3	EDO	D	459	4/4	0.94	0.15	2.12	20,20,24,31	0
2	CL	C	458	1/1	0.97	0.16	1.37	33,33,33,33	0
3	EDO	A	459	4/4	0.95	0.10	1.11	20,23,27,34	0
2	CL	D	458	1/1	0.99	0.11	0.17	24,24,24,24	0
2	CL	A	458	1/1	0.99	0.06	-0.93	23,23,23,23	0
2	CL	B	458	1/1	1.00	0.07	-1.41	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.