



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:01 PM UTC

PDB ID : 6ICM / pdb_00006icm
Title : Pseudomonas putida CBB5 NdmA with ferredoxin domain of NdmD
Authors : Kim, J.H.; Kim, B.H.; Kang, S.Y.; Song, H.K.
Deposited on : 2018-09-06
Resolution : 2.96 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

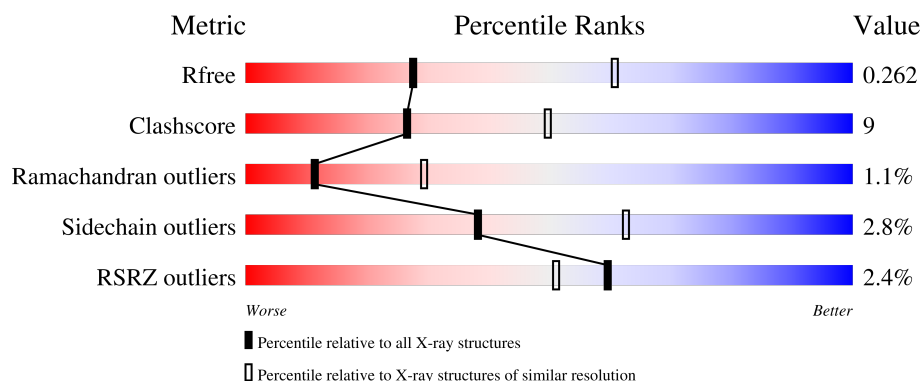
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	369	72% 17% 11%
1	B	369	2% 75% 14% 11%
1	C	369	2% 68% 20% 11%
2	D	87	6% 57% 38% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8753 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 Methylxanthine N1-demethylase NdmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2683	1710	460	501	12			
1	B	330	Total	C	N	O	S	0	0	0
			2682	1710	460	500	12			
1	C	330	Total	C	N	O	S	0	0	0
			2683	1710	460	501	12			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP H9N289
A	-16	GLY	-	expression tag	UNP H9N289
A	-15	SER	-	expression tag	UNP H9N289
A	-14	SER	-	expression tag	UNP H9N289
A	-13	HIS	-	expression tag	UNP H9N289
A	-12	HIS	-	expression tag	UNP H9N289
A	-11	HIS	-	expression tag	UNP H9N289
A	-10	HIS	-	expression tag	UNP H9N289
A	-9	HIS	-	expression tag	UNP H9N289
A	-8	HIS	-	expression tag	UNP H9N289
A	-7	GLU	-	expression tag	UNP H9N289
A	-6	ASN	-	expression tag	UNP H9N289
A	-5	LEU	-	expression tag	UNP H9N289
A	-4	TYR	-	expression tag	UNP H9N289
A	-3	PHE	-	expression tag	UNP H9N289
A	-2	GLN	-	expression tag	UNP H9N289
A	-1	GLY	-	expression tag	UNP H9N289
A	0	SER	-	expression tag	UNP H9N289
B	-17	MET	-	expression tag	UNP H9N289
B	-16	GLY	-	expression tag	UNP H9N289
B	-15	SER	-	expression tag	UNP H9N289
B	-14	SER	-	expression tag	UNP H9N289
B	-13	HIS	-	expression tag	UNP H9N289

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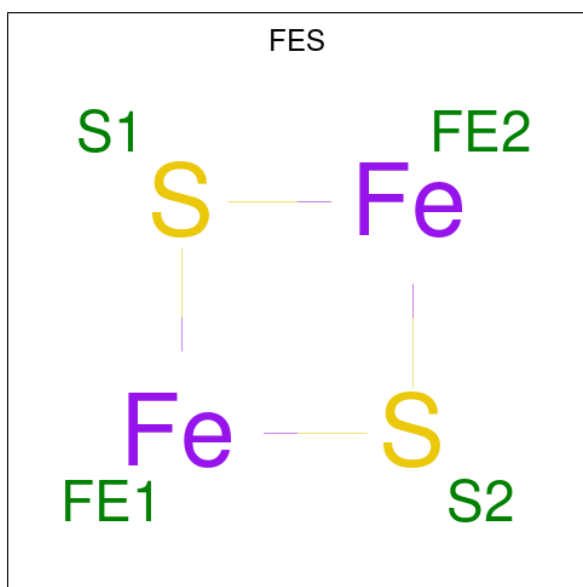
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP H9N289
B	-11	HIS	-	expression tag	UNP H9N289
B	-10	HIS	-	expression tag	UNP H9N289
B	-9	HIS	-	expression tag	UNP H9N289
B	-8	HIS	-	expression tag	UNP H9N289
B	-7	GLU	-	expression tag	UNP H9N289
B	-6	ASN	-	expression tag	UNP H9N289
B	-5	LEU	-	expression tag	UNP H9N289
B	-4	TYR	-	expression tag	UNP H9N289
B	-3	PHE	-	expression tag	UNP H9N289
B	-2	GLN	-	expression tag	UNP H9N289
B	-1	GLY	-	expression tag	UNP H9N289
B	0	SER	-	expression tag	UNP H9N289
C	-17	MET	-	expression tag	UNP H9N289
C	-16	GLY	-	expression tag	UNP H9N289
C	-15	SER	-	expression tag	UNP H9N289
C	-14	SER	-	expression tag	UNP H9N289
C	-13	HIS	-	expression tag	UNP H9N289
C	-12	HIS	-	expression tag	UNP H9N289
C	-11	HIS	-	expression tag	UNP H9N289
C	-10	HIS	-	expression tag	UNP H9N289
C	-9	HIS	-	expression tag	UNP H9N289
C	-8	HIS	-	expression tag	UNP H9N289
C	-7	GLU	-	expression tag	UNP H9N289
C	-6	ASN	-	expression tag	UNP H9N289
C	-5	LEU	-	expression tag	UNP H9N289
C	-4	TYR	-	expression tag	UNP H9N289
C	-3	PHE	-	expression tag	UNP H9N289
C	-2	GLN	-	expression tag	UNP H9N289
C	-1	GLY	-	expression tag	UNP H9N289
C	0	SER	-	expression tag	UNP H9N289

- Molecule 2 is a protein called Oxidoreductase NdmD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	87	Total	C	N	O	S	0	0	0
			670	417	113	133	7			

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

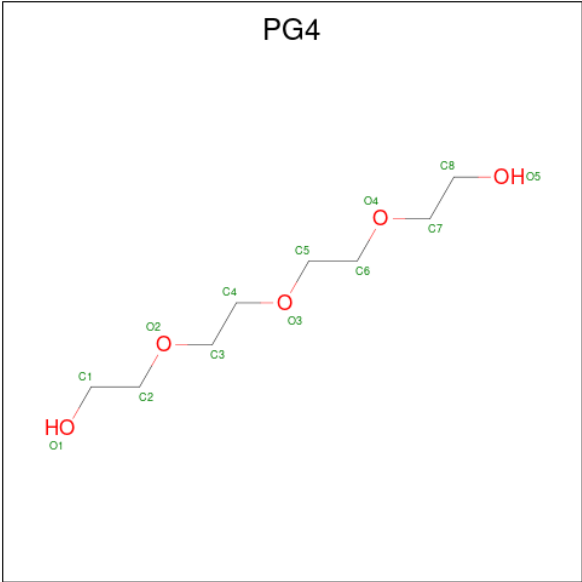


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is water.

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

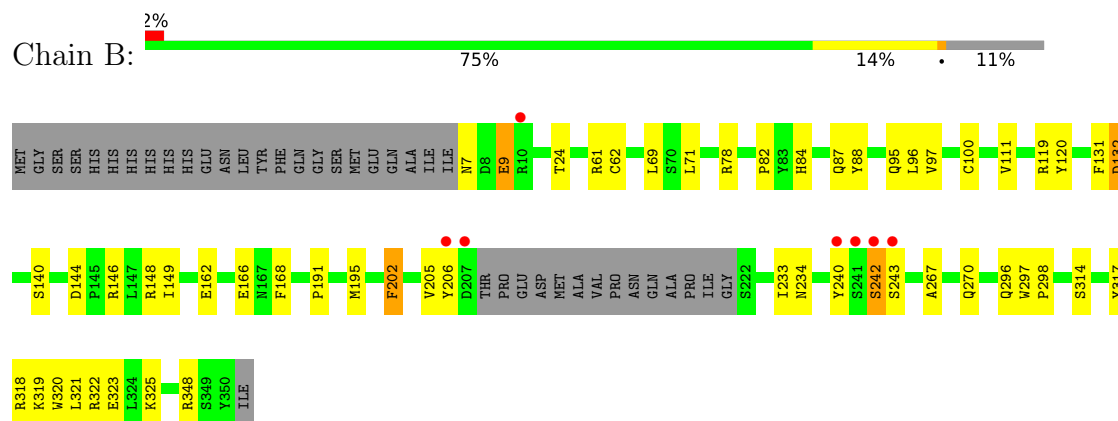
3 Residue-property plots [i](#)

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.

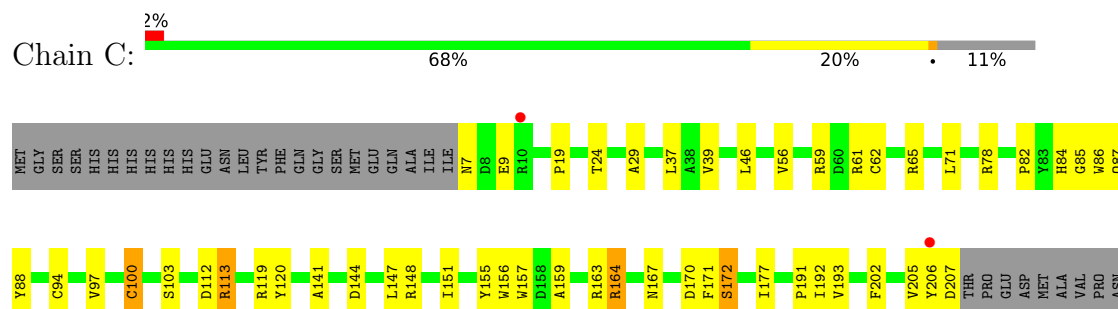
• Molecule 1: Methylxanthine N1-demethylase NdMA



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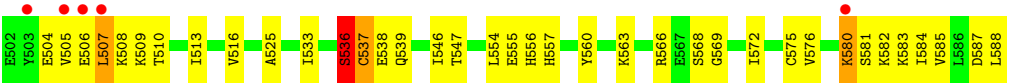


• Molecule 1: Methylxanthine N1-demethylase NdMA





● Molecule 2: Oxidoreductase NdmD



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.27Å 118.27Å 455.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.46 – 2.96 42.46 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.46-2.96) 99.5 (42.46-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.19 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.204 , 0.261 0.208 , 0.262	Depositor DCC
R_{free} test set	2000 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	69.8	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8753	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: FES, FE, PG4

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	0.41	0/2764	0.63	0/3762
1	B	0.45	1/2763 (0.0%)	0.65	0/3761
1	C	0.57	4/2764 (0.1%)	0.60	0/3762
2	D	0.57	0/679	0.85	2/915 (0.2%)
All	All	0.49	5/8970 (0.1%)	0.65	2/12200 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	113	ARG	NE-CZ	-13.84	1.17	1.33
1	C	113	ARG	CD-NE	-12.04	1.29	1.46
1	C	113	ARG	CZ-NH2	-10.08	1.20	1.33
1	C	113	ARG	CZ-NH1	-7.84	1.21	1.32
1	B	9	GLU	CD-OE1	-5.15	1.15	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	580	LYS	CG-CD-CE	-6.39	96.59	111.30
2	D	507	LEU	CA-CB-CG	5.12	134.20	116.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	7	ASN	Peptide

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	2683	0	2545	43	0
1	B	2682	0	2542	38	0
1	C	2683	0	2545	55	0
2	D	670	0	672	36	0
3	A	4	0	0	1	0
3	B	4	0	0	1	0
3	C	4	0	0	1	0
3	D	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	D	13	0	18	4	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
All	All	8753	0	8322	159	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 (159) 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:D:555:GLU:HB2	2:D:580:LYS:NZ	1.70	1.06
2:D:537:CYS:SG	2:D:537:CYS:O	2.15	1.03
1:B:195:MET:HE2	1:B:202:PHE:CE1	2.07	0.89
1:A:268:ARG:NH2	1:A:275:ASP:OD1	2.08	0.86
1:A:268:ARG:NH1	1:A:273:ASP:OD1	2.09	0.85
2:D:555:GLU:HB2	2:D:580:LYS:CE	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLU:O	1:B:325:LYS:NZ	2.13	0.79
2:D:555:GLU:HB2	2:D:580:LYS:HZ2	1.49	0.77
1:C:207:ASP:O	1:C:240:TYR:OH	2.08	0.72
1:B:202:PHE:CE2	1:B:320:TRP:HE3	2.07	0.72
1:A:348:ARG:NH1	1:A:350:TYR:OH	2.23	0.72
1:B:195:MET:HE2	1:B:202:PHE:CD1	2.27	0.70
2:D:555:GLU:HB2	2:D:580:LYS:HZ1	1.57	0.69
2:D:507:LEU:HD12	2:D:583:LYS:HE2	1.75	0.69
2:D:555:GLU:CB	2:D:580:LYS:NZ	2.51	0.68
1:A:89:ASP:OD2	1:A:95:GLN:NE2	2.24	0.68
2:D:555:GLU:HB2	2:D:580:LYS:HE3	1.76	0.68
1:B:84:HIS:NE2	1:C:170:ASP:OD2	2.20	0.65
1:C:159:ALA:O	1:C:260:THR:HG23	1.98	0.64
1:A:172:SER:HB2	1:C:84:HIS:HD2	1.64	0.62
1:B:100:CYS:SG	1:C:309:VAL:HG22	2.39	0.61
1:B:9:GLU:C	1:B:325:LYS:HZ3	2.06	0.61
1:C:157:TRP:CD1	1:C:290:LYS:HD2	2.36	0.61
1:B:314:SER:O	1:B:318:ARG:HG3	2.01	0.60
1:B:144:ASP:OD1	1:B:146:ARG:HD3	2.02	0.60
2:D:555:GLU:OE2	2:D:557:HIS:NE2	2.36	0.59
1:C:192:ILE:HG23	1:C:312:LYS:HD2	1.84	0.58
1:C:336:ARG:HG3	1:C:340:LEU:HD12	1.85	0.58
1:C:206:TYR:HB2	1:C:223:PHE:HB2	1.85	0.58
1:C:29:ALA:HB2	1:C:37:LEU:HD12	1.87	0.56
1:C:164:ARG:O	1:C:164:ARG:HD2	2.04	0.56
1:C:177:ILE:HD11	1:C:289:ASP:OD1	2.05	0.56
1:A:44:GLU:OE1	1:A:59:ARG:NH1	2.38	0.55
2:D:537:CYS:SG	2:D:539:GLN:O	2.64	0.55
1:B:84:HIS:HB2	3:B:400:FES:S1	2.47	0.55
1:A:170:ASP:OD2	1:C:84:HIS:NE2	2.28	0.55
2:D:555:GLU:CB	2:D:580:LYS:HZ1	2.17	0.54
1:C:202:PHE:CE2	1:C:320:TRP:HE3	2.26	0.54
1:B:140:SER:HB3	1:B:234:ASN:HD21	1.73	0.54
1:C:59:ARG:NH1	1:C:112:ASP:OD2	2.30	0.53
2:D:563:LYS:HA	2:D:566:ARG:HG3	1.90	0.53
1:A:314:SER:O	1:A:318:ARG:HG3	2.08	0.53
1:A:20:VAL:HG11	1:A:125:ILE:HD12	1.90	0.53
1:A:139:PHE:HA	1:A:234:ASN:OD1	2.09	0.52
1:B:119:ARG:HG2	1:B:120:TYR:CD2	2.45	0.52
1:B:319:LYS:O	1:B:323:GLU:HG3	2.09	0.52
1:A:297:TRP:HA	1:A:298:PRO:C	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ASP:OD1	1:C:171:PHE:N	2.41	0.52
2:D:555:GLU:CB	2:D:580:LYS:HZ2	2.20	0.52
1:C:242:SER:OG	1:C:243:SER:N	2.42	0.52
1:B:317:TYR:CZ	1:B:321:LEU:HD11	2.46	0.51
2:D:506:GLU:O	2:D:513:ILE:HA	2.11	0.51
1:C:62:CYS:SG	1:C:88:TYR:OH	2.64	0.51
1:B:191:PRO:HG2	1:B:206:TYR:CE1	2.45	0.51
1:C:193:VAL:HG21	1:C:205:VAL:O	2.11	0.51
1:B:322:ARG:NH2	5:D:602:PG4:O1	2.44	0.51
1:A:172:SER:HB2	1:C:84:HIS:CD2	2.45	0.51
2:D:506:GLU:HB2	2:D:584:ILE:O	2.11	0.51
1:A:51:LEU:HD12	1:A:56:VAL:HG21	1.93	0.50
2:D:546:ILE:HD13	5:D:602:PG4:H71	1.93	0.50
1:B:61:ARG:HB2	1:C:297:TRP:CZ2	2.46	0.50
1:A:348:ARG:NH1	1:A:350:TYR:HH	2.08	0.50
2:D:554:LEU:HD22	2:D:572:ILE:HD12	1.94	0.50
1:A:194:PRO:HB2	1:A:346:SER:HB3	1.94	0.50
1:A:177:ILE:HG22	1:A:178:HIS:CE1	2.48	0.49
1:A:239:LYS:HB2	1:A:242:SER:HB3	1.93	0.49
1:B:88:TYR:CE1	1:B:111:VAL:HG13	2.47	0.49
1:B:78:ARG:CZ	1:B:95:GLN:HB2	2.41	0.49
1:B:191:PRO:HG2	1:B:206:TYR:HE1	1.77	0.49
1:B:202:PHE:CE2	1:B:320:TRP:CE3	2.97	0.49
1:B:297:TRP:HA	1:B:298:PRO:C	2.37	0.49
1:B:205:VAL:HG21	1:B:348:ARG:NH2	2.28	0.49
1:C:164:ARG:HD2	1:C:164:ARG:C	2.37	0.49
2:D:546:ILE:CD1	5:D:602:PG4:H71	2.43	0.48
1:C:193:VAL:HG11	1:C:206:TYR:CE1	2.49	0.48
1:B:84:HIS:HD2	1:C:172:SER:HB2	1.79	0.47
2:D:556:HIS:CD2	2:D:566:ARG:HB3	2.48	0.47
1:A:12:TYR:CD1	1:A:325:LYS:HG3	2.50	0.47
1:A:312:LYS:NZ	1:A:345:GLU:OE1	2.47	0.47
1:B:62:CYS:HB2	1:B:69:LEU:HD21	1.97	0.47
1:C:39:VAL:HG23	1:C:46:LEU:HB2	1.97	0.47
2:D:554:LEU:HD12	2:D:569:GLY:HA2	1.96	0.47
2:D:575:CYS:SG	2:D:576:VAL:HG13	2.55	0.46
2:D:508:LYS:HB3	2:D:588:LEU:O	2.15	0.46
1:A:314:SER:HB3	1:C:65:ARG:HH21	1.80	0.46
1:C:100:CYS:HB2	1:C:103:SER:HB2	1.98	0.46
1:C:141:ALA:HB1	1:C:147:LEU:HD12	1.98	0.45
1:B:87:GLN:OE1	1:B:96:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:TRP:NE1	1:C:290:LYS:HD2	2.31	0.45
1:B:9:GLU:C	1:B:325:LYS:NZ	2.71	0.45
1:A:171:PHE:HE1	1:A:313:VAL:HG21	1.82	0.45
1:A:297:TRP:CZ2	1:C:61:ARG:HB2	2.52	0.45
1:C:163:ARG:NH2	1:C:301:ALA:HA	2.31	0.45
1:C:86:TRP:NE1	1:C:97:VAL:HG13	2.32	0.45
1:C:155:TYR:OH	1:C:164:ARG:NH2	2.38	0.44
2:D:516:VAL:HG13	2:D:525:ALA:HB2	1.98	0.44
1:A:171:PHE:HA	1:A:174:PHE:CE2	2.51	0.44
1:B:140:SER:HB3	1:B:234:ASN:ND2	2.32	0.44
1:C:37:LEU:CD2	1:C:39:VAL:HG13	2.47	0.44
1:A:237:VAL:O	1:A:245:LEU:HD12	2.17	0.44
1:B:148:ARG:O	1:B:267:ALA:HA	2.18	0.44
1:B:240:TYR:C	1:B:242:SER:H	2.26	0.44
1:C:113:ARG:HH11	1:C:113:ARG:HD3	1.42	0.44
1:C:297:TRP:HA	1:C:298:PRO:C	2.41	0.44
1:A:100:CYS:HB2	1:A:103:SER:HB2	1.99	0.44
1:C:65:ARG:HB2	3:C:400:FES:S2	2.57	0.44
1:A:162:GLU:O	1:A:166:GLU:HG3	2.17	0.44
1:C:156:TRP:O	1:C:157:TRP:HD1	2.00	0.44
2:D:509:LYS:HG2	2:D:588:LEU:C	2.42	0.44
1:C:19:PRO:O	1:C:253:CYS:HB2	2.18	0.44
2:D:507:LEU:HB3	2:D:585:VAL:HG13	2.00	0.43
1:A:66:SER:O	1:B:296:GLN:HA	2.18	0.43
1:C:245:LEU:HD12	1:C:246:HIS:H	1.84	0.43
2:D:533:ILE:HD11	2:D:547:THR:HG21	2.01	0.43
1:C:245:LEU:N	1:C:269:GLU:OE1	2.47	0.43
1:B:131:PHE:O	1:B:132:ASP:C	2.62	0.43
1:C:167:ASN:ND2	1:C:293:ILE:HD11	2.34	0.43
1:A:245:LEU:HD12	1:A:246:HIS:H	1.83	0.43
1:C:71:LEU:HB2	1:C:82:PRO:HG3	2.01	0.43
1:A:176:PHE:CZ	1:C:85:GLY:HA3	2.53	0.43
1:A:297:TRP:CE2	1:C:61:ARG:HB2	2.54	0.43
5:D:602:PG4:H41	5:D:602:PG4:H62	1.70	0.43
1:C:148:ARG:O	1:C:267:ALA:HA	2.19	0.42
2:D:508:LYS:HB2	2:D:510:THR:HG22	2.00	0.42
1:A:158:ASP:HB3	1:A:294:GLU:HG2	2.00	0.42
1:A:171:PHE:CE1	1:A:313:VAL:HG21	2.55	0.42
2:D:580:LYS:HB2	2:D:580:LYS:HE2	1.79	0.42
2:D:507:LEU:C	2:D:508:LYS:HG2	2.45	0.42
2:D:580:LYS:HE2	2:D:580:LYS:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PHE:HA	1:A:174:PHE:HE2	1.85	0.42
1:A:12:TYR:CE1	1:A:325:LYS:HE2	2.54	0.42
1:C:119:ARG:HG2	1:C:120:TYR:CD2	2.54	0.42
1:B:96:LEU:HD12	1:B:97:VAL:N	2.35	0.42
1:A:314:SER:CB	1:C:65:ARG:HH21	2.33	0.42
1:A:184:ASP:HB3	1:A:187:ASN:HB3	2.02	0.41
1:B:168:PHE:HB3	1:B:233:ILE:HD13	2.01	0.41
1:A:16:PHE:CD1	1:A:230:PRO:HD3	2.55	0.41
1:A:119:ARG:HG2	1:A:120:TYR:CD2	2.55	0.41
1:C:7:ASN:C	1:C:9:GLU:H	2.28	0.41
2:D:505:VAL:HG12	2:D:506:GLU:N	2.35	0.41
1:A:196:ASP:OD2	1:A:348:ARG:NH1	2.53	0.41
1:B:162:GLU:O	1:B:166:GLU:HG3	2.21	0.41
1:B:71:LEU:HB2	1:B:82:PRO:HG3	2.01	0.41
2:D:509:LYS:HE2	2:D:587:ASP:OD1	2.21	0.41
1:B:149:ILE:HG12	1:B:267:ALA:HB2	2.02	0.41
2:D:536:SER:O	2:D:538:GLU:HG3	2.21	0.41
1:A:84:HIS:HB2	3:A:400:FES:S2	2.60	0.41
1:A:242:SER:OG	1:A:244:SER:OG	2.35	0.41
2:D:581:SER:OG	2:D:582:LYS:N	2.54	0.41
1:C:87:GLN:O	1:C:94:CYS:HA	2.21	0.41
1:B:319:LYS:HD2	2:D:560:TYR:CZ	2.56	0.40
1:C:78:ARG:HB3	1:C:88:TYR:O	2.20	0.40
1:C:177:ILE:HG21	1:C:177:ILE:HD13	1.66	0.40
2:D:580:LYS:HZ3	2:D:580:LYS:HG3	1.65	0.40
1:A:163:ARG:NH2	1:A:301:ALA:HA	2.35	0.40
1:A:284:LEU:O	1:A:288:GLU:HG3	2.21	0.40
1:C:191:PRO:HG2	1:C:206:TYR:CE2	2.56	0.40
1:C:151:ILE:HG12	1:C:265:ILE:HG12	2.03	0.40
1:C:312:LYS:NZ	1:C:345:GLU:OE2	2.53	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	326/369 (88%)	301 (92%)	21 (6%)	4 (1%)	10	28
1	B	326/369 (88%)	305 (94%)	17 (5%)	4 (1%)	10	28
1	C	326/369 (88%)	301 (92%)	24 (7%)	1 (0%)	36	59
2	D	85/87 (98%)	74 (87%)	8 (9%)	3 (4%)	3	7
All	All	1063/1194 (89%)	981 (92%)	70 (7%)	12 (1%)	11	29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	SER
1	B	270	GLN
1	A	241	SER
1	B	242	SER
1	A	137	PRO
1	A	242	SER
1	A	270	GLN
2	D	568	SER
2	D	536	SER
1	B	132	ASP
2	D	537	CYS
1	C	144	ASP

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	213/328 (65%)	204 (96%)	9 (4%)	26	53
1	B	158/328 (48%)	156 (99%)	2 (1%)	61	78
1	C	295/328 (90%)	287 (97%)	8 (3%)	39	64
2	D	79/79 (100%)	77 (98%)	2 (2%)	42	66
All	All	745/1063 (70%)	724 (97%)	21 (3%)	38	62

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

Mol	Chain	Res	Type
1	A	100	CYS
1	A	113	ARG
1	A	172	SER
1	A	202	PHE
1	A	207	ASP
1	A	228	SER
1	A	234	ASN
1	A	242	SER
1	A	243	SER
1	B	24	THR
1	B	202	PHE
1	C	24	THR
1	C	56	VAL
1	C	100	CYS
1	C	164	ARG
1	C	172	SER
1	C	222	SER
1	C	255	VAL
1	C	257	SER
2	D	504	GLU
2	D	536	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	199	ASN
1	B	258	HIS
1	C	270	GLN
2	D	524	GLN
2	D	556	HIS

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 8 ligands modelled in this entry, 3 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	FES	C	400	1	0,4,4	-	-	-		
3	FES	A	400	1	0,4,4	-	-	-		
3	FES	B	400	1	0,4,4	-	-	-		
5	PG4	D	602	-	12,12,12	0.54	0	11,11,11	0.45	0
3	FES	D	601	2	0,4,4	-	-	-		

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	FES	C	400	1	-	-	0/1/1/1
3	FES	A	400	1	-	-	0/1/1/1
3	FES	B	400	1	-	-	0/1/1/1
5	PG4	D	602	-	-	5/10/10/10	-
3	FES	D	601	2	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	602	PG4	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
5	D	602	PG4	O2-C3-C4-O3
5	D	602	PG4	O1-C1-C2-O2
5	D	602	PG4	C8-C7-O4-C6
5	D	602	PG4	C1-C2-O2-C3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	400	FES	1	0
3	A	400	FES	1	0
3	B	400	FES	1	0
5	D	602	PG4	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	330/369 (89%)	-0.26	5 (1%) 72 65	38, 53, 88, 128	0
1	B	330/369 (89%)	-0.26	7 (2%) 63 55	37, 53, 87, 123	0
1	C	330/369 (89%)	-0.05	9 (2%) 56 48	48, 65, 101, 136	0
2	D	87/87 (100%)	0.31	5 (5%) 29 24	51, 67, 90, 116	0
All	All	1077/1194 (90%)	-0.15	26 (2%) 59 51	37, 58, 93, 136	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	206	TYR	5.5
1	A	240	TYR	4.9
1	B	206	TYR	4.0
1	C	240	TYR	3.9
2	D	506	GLU	3.3
1	A	239	LYS	3.2
1	B	240	TYR	3.1
2	D	505	VAL	3.1
1	A	242	SER	3.1
1	C	241	SER	3.1
2	D	503	TYR	2.9
1	B	242	SER	2.8
1	B	243	SER	2.7
2	D	507	LEU	2.6
1	B	207	ASP	2.6
1	C	222	SER	2.4
2	D	580	LYS	2.4
1	C	239	LYS	2.4
1	B	241	SER	2.3
1	C	350	TYR	2.2
1	C	242	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	10	ARG	2.2
1	C	243	SER	2.1
1	A	243	SER	2.1
1	A	244	SER	2.0
1	C	10	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	FE	B	401	1/1	0.81	0.16	100,100,100,100	0
5	PG4	D	602	13/13	0.92	0.11	49,54,57,59	0
4	FE	C	401	1/1	0.94	0.15	106,106,106,106	0
4	FE	A	401	1/1	0.95	0.12	95,95,95,95	0
3	FES	D	601	4/4	0.99	0.03	60,64,67,73	0
3	FES	C	400	4/4	1.00	0.02	51,52,53,55	0
3	FES	A	400	4/4	1.00	0.02	39,40,42,43	0
3	FES	B	400	4/4	1.00	0.02	51,52,54,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.