Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 07:56 PM EDT

PDB ID	:	6OZ7
Title	:	Putative oxidoreductase from Escherichia coli str. K-12
Authors	:	Osipiuk, J.; Skarina, T.; Mesa, N.; Endres, M.; Savchenko, A.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2019-05-15
Resolution	:	1.36 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:

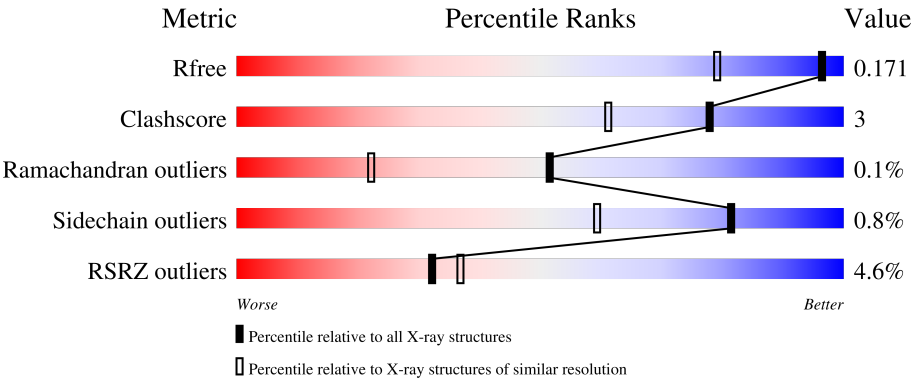
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.36 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}	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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 <=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	254	2% 91% • 5%
1	B	254	2% 83% 9% 7%
1	C	254	9% 87% 7% • 5%
1	D	254	4% 86% 7% 7%
1	E	254	4% 92% • 5%

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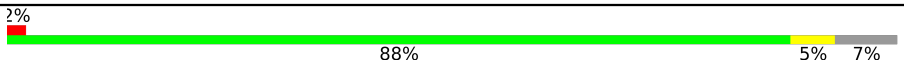
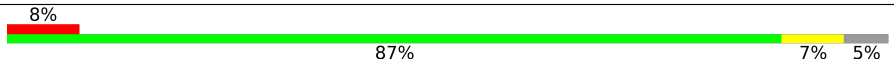
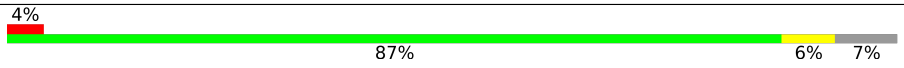
Mol	Chain	Length	Quality of chain
1	F	254	
1	G	254	
1	H	254	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16852 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 Uncharacterized oxidoreductase YohF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	14	0
			1890	1199	326	357	8			
1	B	236	Total	C	N	O	S	0	17	0
			1862	1187	322	345	8			
1	C	241	Total	C	N	O	S	0	13	0
			1878	1195	326	349	8			
1	D	237	Total	C	N	O	S	0	24	0
			1910	1219	326	353	12			
1	E	241	Total	C	N	O	S	0	11	0
			1868	1185	329	345	9			
1	F	237	Total	C	N	O	S	0	17	0
			1861	1189	322	342	8			
1	G	241	Total	C	N	O	S	0	16	0
			1898	1207	327	355	9			
1	H	237	Total	C	N	O	S	0	14	0
			1844	1178	314	340	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P33368
A	1	ASN	-	expression tag	UNP P33368
B	0	SER	-	expression tag	UNP P33368
B	1	ASN	-	expression tag	UNP P33368
C	0	SER	-	expression tag	UNP P33368
C	1	ASN	-	expression tag	UNP P33368
D	0	SER	-	expression tag	UNP P33368
D	1	ASN	-	expression tag	UNP P33368
E	0	SER	-	expression tag	UNP P33368
E	1	ASN	-	expression tag	UNP P33368
F	0	SER	-	expression tag	UNP P33368
F	1	ASN	-	expression tag	UNP P33368
G	0	SER	-	expression tag	UNP P33368

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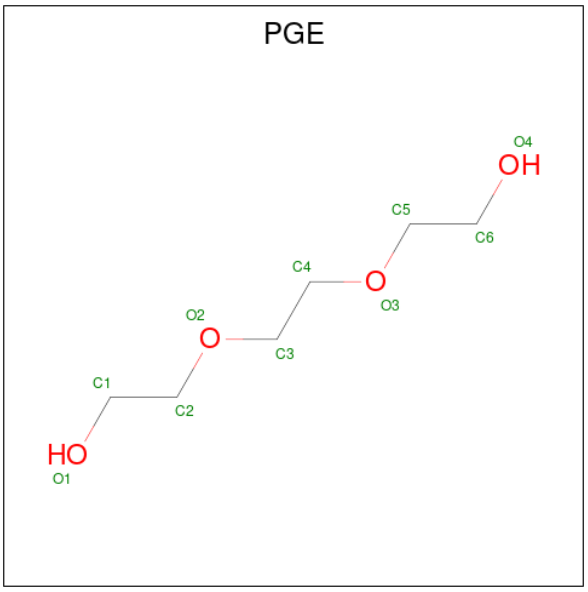
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ASN	-	expression tag	UNP P33368
H	0	SER	-	expression tag	UNP P33368
H	1	ASN	-	expression tag	UNP P33368

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

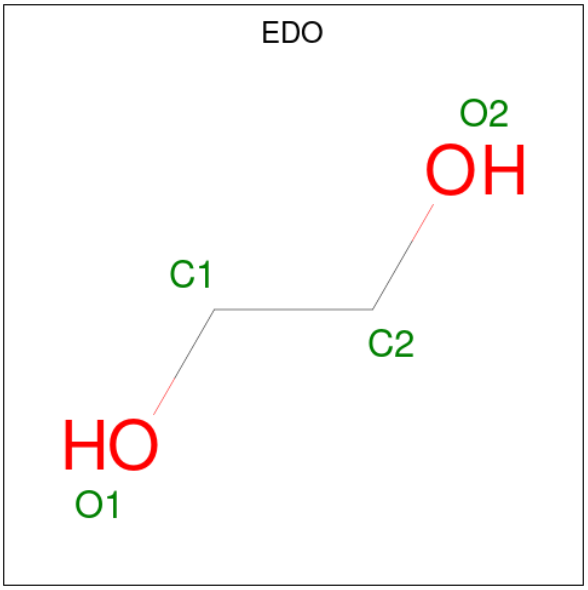
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 10 6 4	0	0
3	D	1	Total C O 10 6 4	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	234	Total O 234 234	0	2
5	B	237	Total O 237 237	0	1
5	C	185	Total O 185 185	0	1
5	D	245	Total O 245 245	0	4
5	E	224	Total O 224 224	0	1

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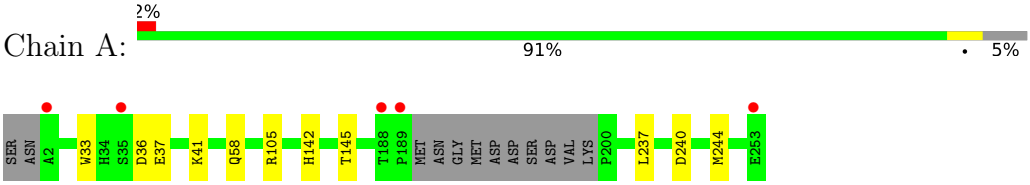
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	222	Total O 222 222	0	3
5	G	194	Total O 195 195	0	2
5	H	259	Total O 259 259	0	3

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.

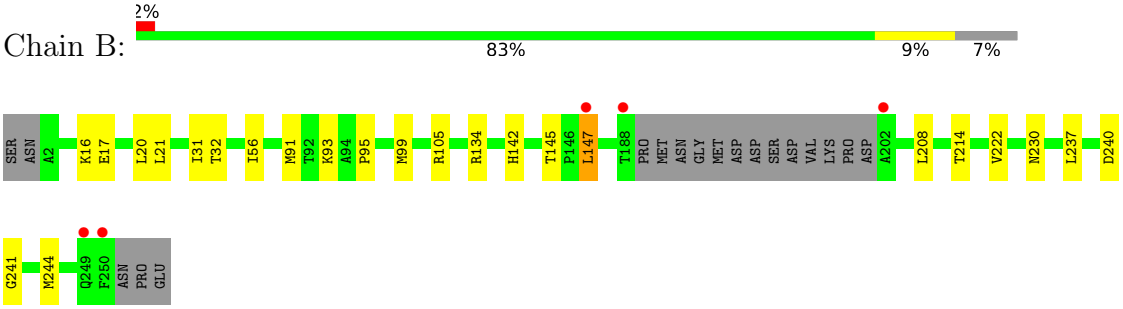
• Molecule 1: Uncharacterized oxidoreductase YohF

Chain A:



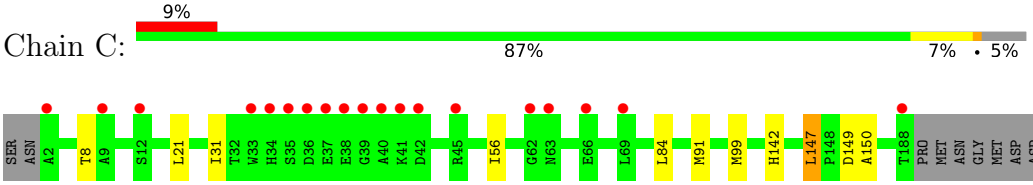
• Molecule 1: Uncharacterized oxidoreductase YohF

Chain B:



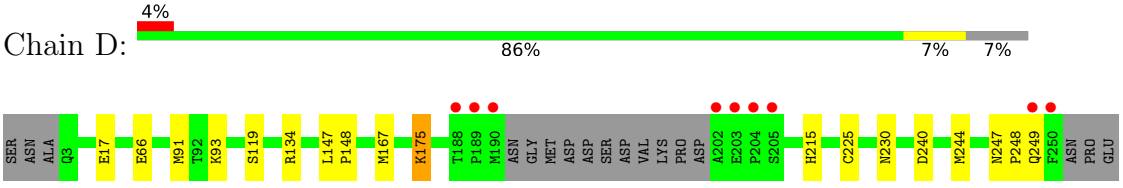
• Molecule 1: Uncharacterized oxidoreductase YohF

Chain C:



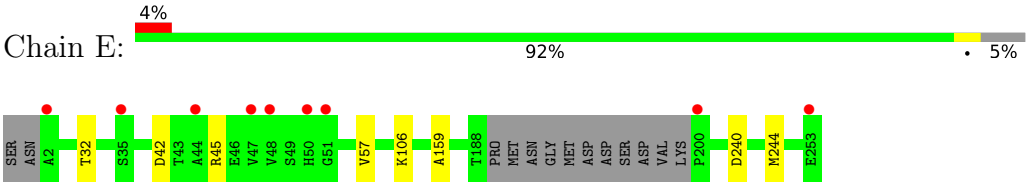
• Molecule 1: Uncharacterized oxidoreductase YohF

Chain D:



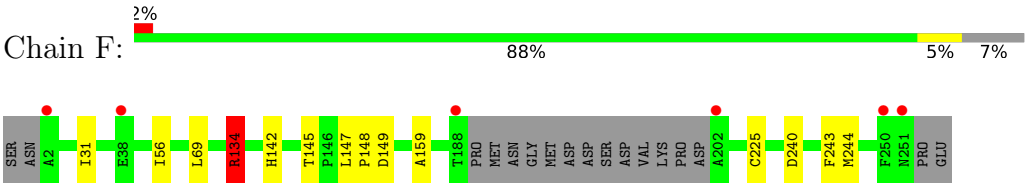
• Molecule 1: Uncharacterized oxidoreductase YohF

Chain E:



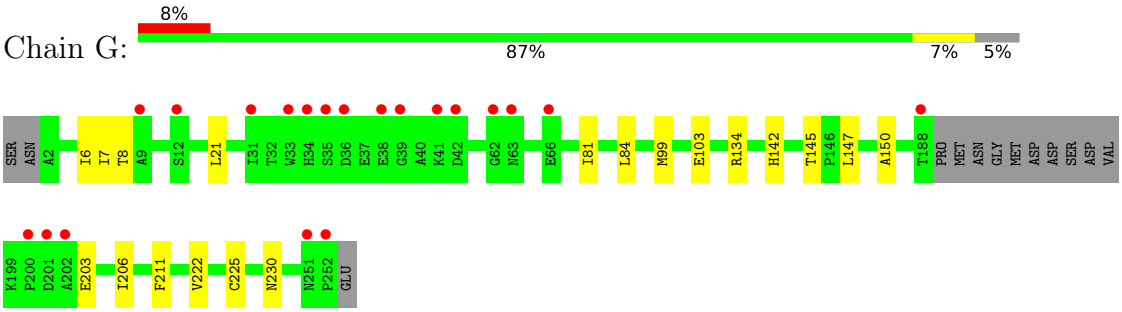
• Molecule 1: Uncharacterized oxidoreductase YohF

Chain F:



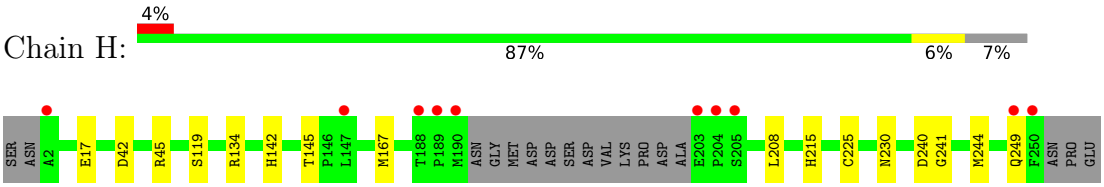
• Molecule 1: Uncharacterized oxidoreductase YohF

Chain G:



• Molecule 1: Uncharacterized oxidoreductase YohF

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.82Å 72.21Å 119.94Å 82.59° 87.03° 67.82°	Depositor
Resolution (Å)	48.14 – 1.36 48.10 – 1.36	Depositor EDS
% Data completeness (in resolution range)	88.1 (48.14-1.36) 88.1 (48.10-1.36)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.36Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.123 , 0.169 0.125 , 0.171	Depositor DCC
R_{free} test set	15748 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	14.9	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	16852	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PGE, EDO, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.69	0/1957	0.79	0/2656
1	B	0.66	0/1937	0.81	0/2626
1	C	0.68	0/1948	0.80	0/2642
1	D	0.70	0/2007	0.81	0/2720
1	E	0.68	0/1933	0.77	0/2617
1	F	0.67	0/1939	0.84	2/2631 (0.1%)
1	G	0.67	0/1970	0.79	0/2673
1	H	0.67	0/1916	0.79	0/2596
All	All	0.68	0/15607	0.80	2/21161 (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	F	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	134[A]	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	F	134[B]	ARG	NE-CZ-NH2	-5.41	117.59	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	147[B]	LEU	Mainchain

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	1890	0	1915	6	0
1	B	1862	0	1915	13	0
1	C	1878	0	1926	13	0
1	D	1910	0	1977	13	0
1	E	1868	0	1916	4	0
1	F	1861	0	1920	16	0
1	G	1898	0	1941	12	0
1	H	1844	0	1907	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	C	10	0	14	0	0
3	D	10	0	14	0	0
4	E	8	0	12	0	0
4	H	4	0	6	0	0
5	A	234	0	0	0	0
5	B	237	0	0	0	1
5	C	185	0	0	0	0
5	D	245	0	0	2	1
5	E	224	0	0	0	0
5	F	222	0	0	2	0
5	G	195	0	0	1	0
5	H	259	0	0	1	0
All	All	16852	0	15463	87	1

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 (87) 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:H:134[A]:ARG:NH2	1:H:230:ASN:OD1	2.36	0.59
1:B:240:ASP:OD2	1:B:244:MET:HG2	2.04	0.57
1:D:247:ASN:HB3	1:D:248:PRO:HD2	1.87	0.55
1:B:142:HIS:CE1	1:B:147[A]:LEU:HD13	2.42	0.55
1:E:42:ASP:OD1	1:E:45:ARG:NH2	2.39	0.55
1:C:149:ASP:OD1	1:C:149:ASP:N	2.40	0.54
1:H:249:GLN:NE2	5:H:405:HOH:O	2.39	0.52
1:F:134[A]:ARG:HH11	1:F:134[A]:ARG:CG	2.23	0.52
1:A:37:GLU:HG2	1:A:41:LYS:HZ2	1.74	0.52
1:D:247:ASN:HB3	1:D:248:PRO:CD	2.41	0.51
1:F:134[A]:ARG:HD3	1:F:225:CYS:HA	1.93	0.51
1:G:134[B]:ARG:NH2	1:G:230:ASN:OD1	2.43	0.50
1:B:91:MET:SD	1:B:93:LYS:HG3	2.51	0.50
1:F:134[A]:ARG:CD	1:F:225:CYS:HA	2.42	0.50
1:F:240:ASP:OD2	1:F:244:MET:HG2	2.12	0.50
1:F:31[B]:ILE:HB	1:F:56[B]:ILE:HG22	1.94	0.49
1:C:142:HIS:CE1	1:C:147[A]:LEU:HD13	2.47	0.49
1:D:134[B]:ARG:NH2	1:D:230:ASN:OD1	2.45	0.49
1:D:17[B]:GLU:HG2	1:D:215[B]:HIS:HA	1.95	0.49
1:D:147[B]:LEU:HD12	1:D:148[B]:PRO:HD2	1.95	0.48
1:G:103[A]:GLU:HG2	5:G:756:HOH:O	2.12	0.48
1:C:203[A]:GLU:HG3	1:C:211:PHE:CZ	2.49	0.47
1:F:149[B]:ASP:CG	5:F:602:HOH:O	2.53	0.47
1:C:240:ASP:OD2	1:C:244:MET:HG2	2.15	0.47
1:F:69[B]:LEU:CD1	5:F:606:HOH:O	2.63	0.46
1:F:134[A]:ARG:HH11	1:F:134[A]:ARG:HG3	1.81	0.46
1:B:17[B]:GLU:HG3	1:B:214:THR:OG1	2.16	0.46
1:B:16:LYS:HE2	1:B:20:LEU:HD11	1.98	0.46
1:H:17[B]:GLU:HG2	1:H:215:HIS:HA	1.96	0.46
1:B:21:LEU:HB3	1:B:222:VAL:HG21	1.97	0.45
1:C:199:LYS:N	1:C:200:PRO:HD2	2.31	0.45
1:C:147[B]:LEU:O	1:C:149:ASP:N	2.50	0.45
1:D:249:GLN:HA	1:D:249:GLN:HE21	1.81	0.45
1:C:21:LEU:HB3	1:C:222:VAL:HG21	1.97	0.45
1:H:208[A]:LEU:HD12	1:H:241:GLY:HA2	1.99	0.45
1:D:240:ASP:OD2	1:D:244:MET:HG2	2.17	0.44
1:H:134[B]:ARG:CD	1:H:225:CYS:HA	2.46	0.44
1:B:142:HIS:HA	1:B:145:THR:O	2.17	0.44
1:B:208[B]:LEU:HD12	1:B:241:GLY:HA2	1.99	0.44
1:H:249:GLN:HA	1:H:249:GLN:HE21	1.81	0.44
1:B:134[A]:ARG:NH2	1:B:230:ASN:OD1	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66[B]:GLU:H	1:D:66[B]:GLU:CD	2.20	0.44
1:H:134[B]:ARG:HD3	1:H:225:CYS:HA	2.00	0.44
1:D:119:SER:HB3	1:D:167[B]:MET:HE1	2.00	0.44
1:D:249:GLN:NE2	5:D:612:HOH:O	2.51	0.44
1:G:147[B]:LEU:HD13	1:G:150:ALA:HB3	2.00	0.44
1:G:203[A]:GLU:HG3	1:G:206[A]:ILE:HG12	1.99	0.44
1:H:240:ASP:OD2	1:H:244:MET:HG2	2.18	0.44
1:G:134[A]:ARG:CD	1:G:225:CYS:HA	2.48	0.43
1:G:147[B]:LEU:CD1	1:G:150:ALA:HB3	2.47	0.43
1:A:240:ASP:OD2	1:A:244:MET:HG2	2.18	0.43
1:C:247:ASN:HB2	1:C:248:PRO:CD	2.49	0.43
1:G:6:ILE:HD12	1:G:81:ILE:HD12	2.00	0.43
1:D:134[A]:ARG:HD3	1:D:225:CYS:HA	2.01	0.43
1:A:142:HIS:HA	1:A:145:THR:O	2.19	0.43
1:G:21:LEU:HB3	1:G:222:VAL:HG21	2.00	0.42
1:A:33:TRP:CZ2	1:A:58:GLN:HB2	2.53	0.42
1:F:134[A]:ARG:CG	1:F:134[A]:ARG:NH1	2.82	0.42
1:C:199:LYS:N	1:C:200:PRO:CD	2.83	0.42
1:G:8:THR:HG23	1:G:84:LEU:HD11	2.01	0.42
1:B:147[A]:LEU:HD12	1:B:147[A]:LEU:HA	1.78	0.42
1:F:149[A]:ASP:OD1	1:F:149[A]:ASP:N	2.52	0.42
1:H:42[A]:ASP:OD1	1:H:45:ARG:NH2	2.52	0.42
1:H:142:HIS:HA	1:H:145:THR:O	2.20	0.42
1:D:91[B]:MET:SD	1:D:93:LYS:HG3	2.59	0.42
1:G:142:HIS:HA	1:G:145:THR:O	2.20	0.42
1:G:203[B]:GLU:HG3	1:G:211:PHE:CZ	2.55	0.42
1:C:91:MET:CE	1:C:147[B]:LEU:HD11	2.50	0.41
1:E:240:ASP:OD2	1:E:244:MET:HG2	2.20	0.41
1:B:95:PRO:HG3	5:D:814:HOH:O	2.20	0.41
1:E:32:THR:HA	1:E:57:VAL:O	2.21	0.41
1:C:147[B]:LEU:HB3	1:C:150:ALA:HB3	2.02	0.41
1:D:175:LYS:HD2	1:D:175:LYS:N	2.36	0.41
1:F:142:HIS:HA	1:F:145:THR:O	2.21	0.41
1:B:31:ILE:HB	1:B:56[B]:ILE:HG22	2.04	0.40
1:E:159:ALA:HB2	1:F:159:ALA:HB2	2.03	0.40
1:F:243:PHE:CZ	1:H:249:GLN:HG2	2.56	0.40
1:A:37:GLU:HG2	1:A:41:LYS:NZ	2.36	0.40
1:H:119:SER:HB3	1:H:167[B]:MET:HE1	2.04	0.40
1:C:8:THR:HG23	1:C:84:LEU:HD11	2.04	0.40
1:C:31:ILE:HB	1:C:56:ILE:HG22	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:697:HOH:O	5:D:716:HOH:O[1_565]	2.07	0.13

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	252/254 (99%)	241 (96%)	9 (4%)	2 (1%)	19 3
1	B	249/254 (98%)	242 (97%)	7 (3%)	0	100 100
1	C	250/254 (98%)	238 (95%)	12 (5%)	0	100 100
1	D	257/254 (101%)	244 (95%)	13 (5%)	0	100 100
1	E	248/254 (98%)	242 (98%)	6 (2%)	0	100 100
1	F	250/254 (98%)	241 (96%)	9 (4%)	0	100 100
1	G	253/254 (100%)	243 (96%)	10 (4%)	0	100 100
1	H	247/254 (97%)	240 (97%)	7 (3%)	0	100 100
All	All	2006/2032 (99%)	1931 (96%)	73 (4%)	2 (0%)	51 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36[A]	ASP
1	A	36[B]	ASP

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	201/198 (102%)	200 (100%)	1 (0%)	88 74
1	B	198/198 (100%)	192 (97%)	6 (3%)	41 9
1	C	199/198 (100%)	195 (98%)	4 (2%)	55 21
1	D	207/198 (104%)	206 (100%)	1 (0%)	88 74
1	E	197/198 (100%)	195 (99%)	2 (1%)	76 49
1	F	199/198 (100%)	197 (99%)	2 (1%)	76 49
1	G	202/198 (102%)	201 (100%)	1 (0%)	88 74
1	H	197/198 (100%)	197 (100%)	0	100 100
All	All	1600/1584 (101%)	1583 (99%)	17 (1%)	81 45

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	B	32	THR
1	B	99	MET
1	B	105[A]	ARG
1	B	105[B]	ARG
1	B	147[A]	LEU
1	B	147[B]	LEU
1	C	99	MET
1	C	147[A]	LEU
1	C	147[B]	LEU
1	C	199	LYS
1	D	175	LYS
1	E	106[A]	LYS
1	E	106[B]	LYS
1	F	134[A]	ARG
1	F	134[B]	ARG
1	G	99	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	249	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 8 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	PGE	C	502	-	9,9,9	0.33	0	8,8,8	0.14	0
4	EDO	E	502	-	3,3,3	0.35	0	2,2,2	0.32	0
4	EDO	E	503	-	3,3,3	0.33	0	2,2,2	0.20	0
4	EDO	H	301	-	3,3,3	0.21	0	2,2,2	0.06	0
3	PGE	D	502	-	9,9,9	0.19	0	8,8,8	0.09	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	PGE	C	502	-	-	0/7/7/7	-
4	EDO	E	502	-	-	0/1/1/1	-
4	EDO	E	503	-	-	0/1/1/1	-
4	EDO	H	301	-	-	1/1/1/1	-
3	PGE	D	502	-	-	4/7/7/7	-

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
3	D	502	PGE	O1-C1-C2-O2
4	H	301	EDO	O1-C1-C2-O2
3	D	502	PGE	C1-C2-O2-C3
3	D	502	PGE	O3-C5-C6-O4
3	D	502	PGE	O2-C3-C4-O3

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	242/254 (95%)	0.16	5 (2%)	63	69	10, 16, 31, 55	0
1	B	236/254 (92%)	0.17	5 (2%)	63	69	10, 16, 30, 45	0
1	C	241/254 (94%)	0.45	23 (9%)	8	10	11, 18, 38, 54	0
1	D	237/254 (93%)	0.29	9 (3%)	40	45	11, 17, 33, 67	0
1	E	241/254 (94%)	0.27	9 (3%)	41	47	10, 17, 38, 63	0
1	F	237/254 (93%)	0.25	6 (2%)	57	63	11, 17, 31, 58	0
1	G	241/254 (94%)	0.45	20 (8%)	11	12	11, 19, 37, 59	0
1	H	237/254 (93%)	0.22	10 (4%)	36	41	11, 17, 33, 52	0
All	All	1912/2032 (94%)	0.28	87 (4%)	32	37	10, 17, 35, 67	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	189	PRO	8.4
1	C	200	PRO	7.2
1	D	189	PRO	6.9
1	C	202	ALA	6.9
1	C	33	TRP	5.7
1	D	204	PRO	5.5
1	G	200	PRO	5.4
1	H	190	MET	5.4
1	E	2	ALA	5.3
1	D	190	MET	5.2
1	A	188	THR	5.2
1	C	38	GLU	4.7
1	G	33	TRP	4.6
1	G	202	ALA	4.4
1	G	38	GLU	4.4
1	D	205	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	202	ALA	4.1
1	G	66[A]	GLU	4.1
1	D	188	THR	4.1
1	C	201	ASP	3.9
1	G	9	ALA	3.9
1	E	200	PRO	3.8
1	A	35[A]	SER	3.8
1	G	251	ASN	3.8
1	H	204	PRO	3.8
1	C	63	ASN	3.6
1	G	36	ASP	3.6
1	C	9	ALA	3.6
1	E	253	GLU	3.5
1	B	250	PHE	3.4
1	E	51	GLY	3.4
1	E	48	VAL	3.4
1	G	34	HIS	3.4
1	D	203[A]	GLU	3.3
1	G	35	SER	3.3
1	A	253	GLU	3.3
1	G	188	THR	3.2
1	H	188	THR	3.2
1	C	35	SER	3.2
1	E	50	HIS	3.2
1	F	250	PHE	3.1
1	E	44	ALA	3.1
1	B	188	THR	3.1
1	C	45	ARG	3.0
1	G	201	ASP	3.0
1	C	34	HIS	2.9
1	A	2	ALA	2.9
1	G	42	ASP	2.8
1	G	39	GLY	2.8
1	A	189	PRO	2.8
1	H	250	PHE	2.8
1	H	2	ALA	2.8
1	F	251	ASN	2.7
1	C	12	SER	2.7
1	B	147[A]	LEU	2.7
1	C	188	THR	2.7
1	G	31	ILE	2.7
1	B	202	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	42	ASP	2.6
1	F	202	ALA	2.6
1	C	2	ALA	2.6
1	H	205	SER	2.6
1	F	188	THR	2.5
1	E	35	SER	2.5
1	G	12	SER	2.5
1	C	66	GLU	2.4
1	C	62	GLY	2.4
1	C	37	GLU	2.4
1	C	39	GLY	2.4
1	C	41	LYS	2.3
1	C	199	LYS	2.3
1	C	36	ASP	2.3
1	H	249	GLN	2.3
1	D	250	PHE	2.3
1	F	38[A]	GLU	2.3
1	G	252	PRO	2.2
1	F	2	ALA	2.2
1	E	47	VAL	2.2
1	B	249	GLN	2.2
1	G	41[A]	LYS	2.2
1	C	69	LEU	2.1
1	C	40	ALA	2.1
1	D	249	GLN	2.1
1	G	62	GLY	2.1
1	G	63	ASN	2.1
1	H	147	LEU	2.1
1	H	203	GLU	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 monosaccharides 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, 95^{th} 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	PGE	D	502	10/10	0.85	0.19	31,40,49,54	0
3	PGE	C	502	10/10	0.87	0.12	21,39,51,56	0
4	EDO	E	503	4/4	0.89	0.11	25,29,30,40	0
4	EDO	E	502	4/4	0.95	0.12	22,25,31,42	0
2	CA	G	501	1/1	0.95	0.08	32,32,32,32	1
4	EDO	H	301	4/4	0.96	0.06	30,32,36,40	0
2	CA	C	501	1/1	0.97	0.11	31,31,31,31	1
2	CA	F	501	1/1	0.98	0.06	24,24,24,24	1
2	CA	E	501	1/1	0.99	0.04	31,31,31,31	1
2	CA	B	501	1/1	0.99	0.06	28,28,28,28	1
2	CA	H	302	1/1	1.00	0.05	17,17,17,17	0
2	CA	D	501	1/1	1.00	0.06	17,17,17,17	1
2	CA	A	501	1/1	1.00	0.04	18,18,18,18	1

6.5 Other polymers (i)

There are no such residues in this entry.