



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:43 am BST

PDB ID : 5LXO
Title : Coiled-coil protein
Authors : Thiyagarajan, N.; Bunney, T.D.; Katan, M.
Deposited on : 2016-09-22
Resolution : 2.18 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 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 : 2.11
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) : 2.11

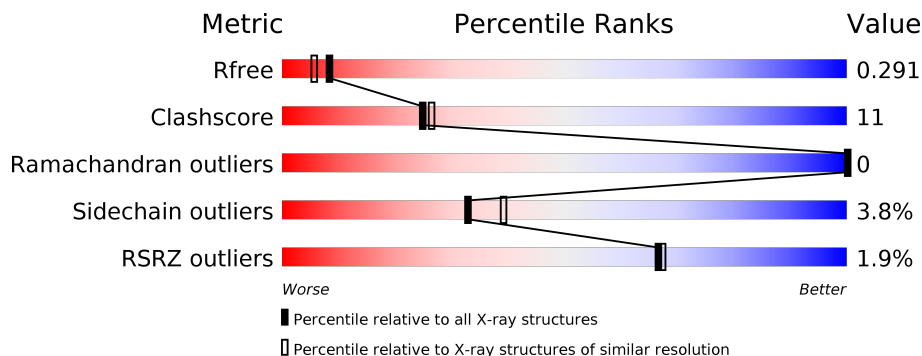
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 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	81	
1	B	81	
1	C	81	
1	D	81	
1	E	81	
1	F	81	

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Mol	Chain	Length	Quality of chain
1	G	81	
1	H	81	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	B	903	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5627 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 Transforming acidic coiled-coil-containing protein 3.

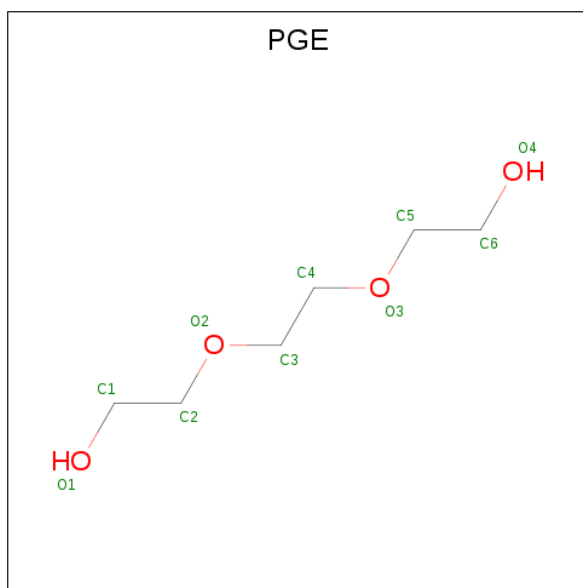
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	80	Total 651	C 396	N 119	O 132	S 1	Se 3	0	1	0
1	B	80	Total 658	C 404	N 119	O 130	S 2	Se 3	0	3	0
1	C	81	Total 677	C 413	N 123	O 137	S 1	Se 3	0	3	0
1	D	77	Total 635	C 387	N 115	O 129	S 1	Se 3	0	3	0
1	E	81	Total 672	C 411	N 123	O 135	S 1	Se 2	0	3	0
1	F	77	Total 626	C 381	N 114	O 127	S 1	Se 3	0	1	0
1	G	80	Total 646	C 393	N 118	O 131	S 2	Se 2	0	1	0
1	H	78	Total 645	C 397	N 116	O 126	S 2	Se 4	0	4	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



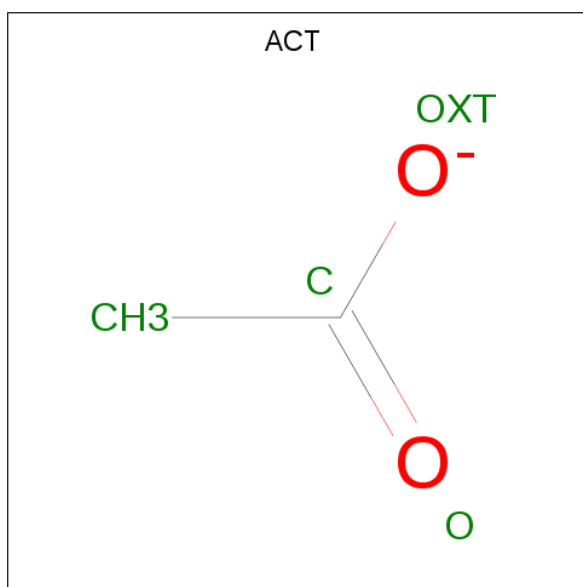
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

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



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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	56	Total O 56 56	0	0
6	B	48	Total O 48 48	0	0
6	C	57	Total O 57 57	0	0
6	D	41	Total O 41 41	0	0
6	E	39	Total O 39 39	0	0
6	F	32	Total O 32 32	0	0
6	G	58	Total O 58 58	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	56	Total	O	0	0
			56	56		

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: Transforming acidic coiled-coil-containing protein 3

Chain A: 




- Molecule 1: Transforming acidic coiled-coil-containing protein 3

Chain B: 



- Molecule 1: Transforming acidic coiled-coil-containing protein 3

Chain C: 



- Molecule 1: Transforming acidic coiled-coil-containing protein 3

Chain D: 



- Molecule 1: Transforming acidic coiled-coil-containing protein 3

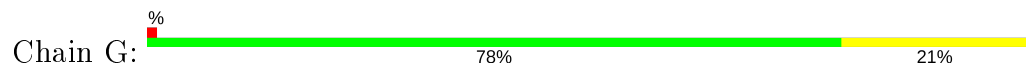
Chain E: 



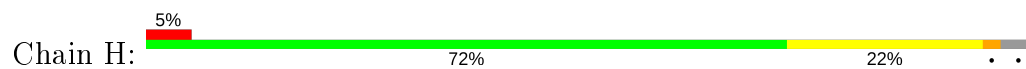
- Molecule 1: Transforming acidic coiled-coil-containing protein 3



- Molecule 1: Transforming acidic coiled-coil-containing protein 3



- Molecule 1: Transforming acidic coiled-coil-containing protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.25Å 76.46Å 86.89Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	28.96 – 2.18 28.96 – 2.18	Depositor EDS
% Data completeness (in resolution range)	95.5 (28.96-2.18) 95.3 (28.96-2.18)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.18Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.233 , 0.285 0.244 , 0.291	Depositor DCC
R_{free} test set	1774 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtrriage
Anisotropy	1.078	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.168 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5627	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.73% 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: CL, PGE, SO4, ACT

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	0.44	0/650	0.60	0/861
1	B	0.42	0/666	0.57	0/881
1	C	0.39	0/676	0.57	0/895
1	D	0.37	0/640	0.47	0/848
1	E	0.38	0/677	0.59	0/897
1	F	0.38	0/625	0.47	0/828
1	G	0.43	0/648	0.54	0/859
1	H	0.34	0/656	0.53	0/868
All	All	0.39	0/5238	0.55	0/6937

There are no bond length outliers.

There are no bond angle outliers.

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	651	0	667	8	0
1	B	658	0	690	18	0
1	C	677	0	695	16	0
1	D	635	0	652	27	1
1	E	672	0	698	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	626	0	639	22	0
1	G	646	0	663	11	1
1	H	645	0	679	20	0
2	B	5	0	0	0	0
3	B	10	0	14	1	0
3	E	10	0	14	0	0
4	B	4	0	3	3	0
5	D	1	0	0	0	0
6	A	56	0	0	2	0
6	B	48	0	0	4	0
6	C	57	0	0	4	0
6	D	41	0	0	4	0
6	E	39	0	0	3	0
6	F	32	0	0	6	0
6	G	58	0	0	1	0
6	H	56	0	0	4	0
All	All	5627	0	5414	115	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 11.

All (115) 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:E:762:GLN:HA	1:E:762:GLN:HE21	1.16	1.07
1:E:765:GLN:NE2	6:E:1001:HOH:O	1.87	1.05
1:F:762:GLN:NE2	6:F:901:HOH:O	2.06	0.87
1:E:829:ASP:OD1	1:H:802:LYS:NZ	2.06	0.87
1:H:823:GLU:OE1	1:H:826:ARG:NH1	2.14	0.80
4:B:903:ACT:O	6:B:1001:HOH:O	2.00	0.79
1:E:762:GLN:HA	1:E:762:GLN:NE2	1.96	0.78
1:A:806:ARG:HG3	1:A:806:ARG:HH11	1.47	0.78
1:H:828[B]:CYS:SG	6:H:941:HOH:O	2.44	0.75
1:C:817:LYS:HE3	1:D:818:THR:HG22	1.69	0.74
1:G:807:ILE:HG13	1:H:807:ILE:HD13	1.69	0.73
1:D:762:GLN:OE1	1:E:838:ILE:HG12	1.90	0.71
1:E:768:LYS:HB2	1:F:767:LEU:HD21	1.73	0.71
1:H:763:ARG:NH1	6:H:902:HOH:O	2.23	0.71
1:F:817:LYS:O	1:F:821:ASN:ND2	2.23	0.70
1:E:758:THR:HG23	1:E:761:GLY:H	1.57	0.69
1:G:786:ARG:NH1	6:G:901:HOH:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:CYS:SG	6:B:1027:HOH:O	2.51	0.67
1:B:816:GLN:HG2	4:B:903:ACT:H1	1.75	0.66
1:G:807:ILE:HG13	1:H:807:ILE:CD1	2.26	0.66
1:D:801:ARG:NH1	6:D:1001:HOH:O	2.24	0.65
1:A:829:ASP:OD1	1:D:802:LYS:NZ	2.27	0.64
1:C:776:GLN:NE2	6:C:903:HOH:O	2.31	0.64
1:B:838:ILE:HD11	1:D:794:LEU:HD12	1.80	0.64
1:G:786:ARG:NH1	1:H:781:GLU:OE2	2.29	0.63
1:F:773:GLU:OE2	6:F:902:HOH:O	2.16	0.61
1:D:770:HIS:CE1	1:F:828:CYS:HB3	2.36	0.60
1:E:785:VAL:HA	1:E:788:LYS:HE2	1.84	0.60
1:B:831:LEU:O	1:B:835[B]:MSE:HG2	2.02	0.59
1:E:838:ILE:HG22	1:E:838:ILE:O	2.00	0.59
1:D:815:GLU:O	1:D:818:THR:OG1	2.15	0.59
1:F:819:LYS:O	1:F:823:GLU:HG3	2.02	0.59
1:B:788:LYS:NZ	1:B:792:GLU:OE2	2.35	0.59
1:C:817:LYS:HA	1:C:820:GLU:HG2	1.85	0.59
1:A:806:ARG:HD3	1:B:807:ILE:HD12	1.85	0.58
1:D:779:ASN:O	1:D:782:ILE:HG22	2.03	0.58
1:G:796:LEU:HD23	1:H:796:LEU:HB3	1.86	0.58
1:E:828:CYS:HB3	1:H:802:LYS:NZ	2.18	0.58
1:B:812:LYS:O	1:B:815:GLU:HG2	2.03	0.58
1:F:819:LYS:O	1:F:822:GLU:HG2	2.03	0.58
1:B:788:LYS:HD3	1:C:838:ILE:HA	1.85	0.57
1:E:772:GLU:OE2	6:E:1002:HOH:O	2.17	0.57
1:A:806:ARG:HG3	1:A:806:ARG:NH1	2.16	0.57
1:E:762:GLN:CA	1:E:762:GLN:HE21	2.03	0.56
1:D:823:GLU:HG2	1:D:826:ARG:HH21	1.70	0.56
4:B:903:ACT:OXT	6:B:1002:HOH:O	2.17	0.56
1:B:790:GLN:HE22	1:D:836:GLU:HA	1.70	0.55
1:D:812:LYS:NZ	6:D:1007:HOH:O	2.40	0.55
1:C:774:LYS:NZ	6:C:904:HOH:O	2.33	0.55
1:H:821:ASN:OD1	6:H:901:HOH:O	2.18	0.55
1:D:770:HIS:HE1	1:F:828:CYS:HB3	1.72	0.54
1:E:782:ILE:HG13	1:F:782:ILE:HG13	1.88	0.54
1:B:823:GLU:HB3	1:D:805[B]:MSE:HE2	1.90	0.53
1:G:760:GLU:HG2	1:G:764:TYR:CE2	2.44	0.53
1:C:761:GLY:O	1:C:765:GLN:OE1	2.27	0.53
1:G:806:ARG:HG3	1:H:807:ILE:HD12	1.91	0.53
1:E:831:LEU:HD21	1:F:831:LEU:HD22	1.90	0.52
1:D:786:ARG:O	1:D:790:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:765:GLN:NE2	1:B:768[B]:LYS:NZ	2.58	0.52
1:G:828[B]:CYS:SG	6:H:941:HOH:O	2.57	0.52
1:C:812[B]:LYS:NZ	6:C:905:HOH:O	2.43	0.51
1:F:834:LYS:NZ	6:F:907:HOH:O	2.42	0.51
1:A:819:LYS:NZ	6:A:904:HOH:O	2.43	0.51
1:H:770:HIS:CE1	1:H:774:LYS:HE3	2.46	0.51
1:C:775:LEU:HD11	1:D:774:LYS:HE3	1.94	0.50
1:D:821:ASN:ND2	6:D:1006:HOH:O	2.38	0.50
1:C:793:ALA:O	1:C:797:GLN:HG2	2.13	0.49
1:C:811:GLU:OE2	1:D:806:ARG:NH2	2.44	0.49
1:C:812[B]:LYS:NZ	6:C:906:HOH:O	2.44	0.48
1:A:788:LYS:HE2	1:A:792:GLU:OE2	2.12	0.48
1:B:823:GLU:HG3	1:B:826:ARG:HH21	1.79	0.48
1:F:805[A]:MSE:HE3	1:H:827:ILE:HD12	1.96	0.47
1:D:822:GLU:O	1:D:825:THR:HG22	2.13	0.47
1:F:817:LYS:NZ	6:F:908:HOH:O	2.46	0.47
1:E:797:GLN:HG3	6:E:1031:HOH:O	2.15	0.46
1:E:819:LYS:HD2	1:E:819:LYS:HA	1.50	0.46
1:E:828:CYS:HB3	1:H:802:LYS:HZ3	1.79	0.45
1:G:767:LEU:O	1:G:770:HIS:HB3	2.16	0.45
1:A:802:LYS:O	1:A:805[B]:MSE:HB2	2.17	0.45
1:B:768[A]:LYS:HE2	1:B:772:GLU:OE2	2.16	0.45
1:H:770:HIS:ND1	1:H:774:LYS:HE3	2.32	0.45
1:D:814:VAL:O	1:D:818:THR:HG23	2.17	0.45
1:B:838:ILE:HD11	1:D:794:LEU:CD1	2.48	0.44
1:C:767:LEU:HD23	1:D:767:LEU:HD23	2.00	0.43
1:H:806:ARG:HE	1:H:806:ARG:HB2	1.57	0.43
1:H:835[A]:MSE:HB3	1:H:835[A]:MSE:HE3	1.78	0.43
1:C:781:GLU:O	1:C:785:VAL:HG13	2.19	0.43
6:A:917:HOH:O	1:E:805:MSE:HG3	2.19	0.43
1:D:770:HIS:HB3	1:F:832:ILE:HD11	2.01	0.43
1:B:818:THR:O	1:B:822:GLU:HG2	2.19	0.42
1:B:800:LEU:O	1:B:804:GLN:HG3	2.20	0.42
3:B:902:PGE:O1	6:B:1003:HOH:O	2.20	0.42
1:E:824:LEU:HB3	1:F:824:LEU:HD23	2.02	0.42
1:D:812:LYS:HE3	1:D:812:LYS:HB2	1.83	0.42
1:B:765:GLN:NE2	1:B:768[B]:LYS:CE	2.82	0.42
1:F:821:ASN:HB3	6:F:928:HOH:O	2.18	0.42
1:F:802:LYS:NZ	6:F:909:HOH:O	2.52	0.42
1:F:835:MSE:HA	1:H:794:LEU:HD11	2.01	0.42
1:C:796:LEU:HD13	1:D:796:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:782:ILE:HA	1:D:785:VAL:HG12	2.03	0.41
1:C:832:ILE:O	1:C:836:GLU:HG2	2.20	0.41
1:E:759:GLN:HA	1:E:762:GLN:HB2	2.03	0.41
1:B:765:GLN:HE21	1:B:768[B]:LYS:CE	2.34	0.41
1:D:813:THR:N	6:D:1008:HOH:O	2.53	0.41
1:E:817[B]:LYS:NZ	1:F:818:THR:OG1	2.53	0.41
1:F:819:LYS:HA	1:F:819:LYS:HD2	1.68	0.41
1:G:768:LYS:O	1:G:772:GLU:HB2	2.21	0.41
1:C:804:GLN:O	1:C:808:GLN:HG3	2.22	0.40
1:D:823:GLU:HG2	1:D:826:ARG:NH2	2.32	0.40
1:E:823:GLU:O	1:E:826:ARG:HB3	2.22	0.40
1:F:816:GLN:O	1:F:820:GLU:HG3	2.22	0.40
1:G:799:SER:O	1:G:803:GLU:HG2	2.21	0.40
1:H:773:GLU:O	1:H:777:LEU:HG	2.21	0.40
1:F:824:LEU:HD13	1:H:805[A]:MSE:HE1	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:834:LYS:NZ	1:G:805:MSE:O[1_456]	2.17	0.03

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	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
1	B	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
1	C	82/81 (101%)	80 (98%)	2 (2%)	0	100	100
1	D	78/81 (96%)	77 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	82/81 (101%)	81 (99%)	1 (1%)	0	100	100
1	F	76/81 (94%)	76 (100%)	0	0	100	100
1	G	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
1	H	80/81 (99%)	77 (96%)	3 (4%)	0	100	100
All	All	637/648 (98%)	624 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	70/68 (103%)	69 (99%)	1 (1%)	67	78
1	B	72/68 (106%)	68 (94%)	4 (6%)	21	23
1	C	73/68 (107%)	73 (100%)	0	100	100
1	D	69/68 (102%)	64 (93%)	5 (7%)	14	14
1	E	73/68 (107%)	70 (96%)	3 (4%)	30	36
1	F	67/68 (98%)	65 (97%)	2 (3%)	41	49
1	G	70/68 (103%)	67 (96%)	3 (4%)	29	34
1	H	71/68 (104%)	67 (94%)	4 (6%)	21	23
All	All	565/544 (104%)	543 (96%)	22 (4%)	33	38

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

Mol	Chain	Res	Type
1	A	787	SER
1	B	773	GLU
1	B	808	GLN
1	B	828[A]	CYS
1	B	828[B]	CYS
1	D	772	GLU

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Mol	Chain	Res	Type
1	D	800	LEU
1	D	825	THR
1	D	834	LYS
1	D	836	GLU
1	E	762	GLN
1	E	808	GLN
1	E	833	SER
1	F	803	GLU
1	F	832	ILE
1	G	788	LYS
1	G	794	LEU
1	G	816	GLN
1	H	762	GLN
1	H	804	GLN
1	H	806	ARG
1	H	826	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	765	GLN
1	B	790	GLN
1	C	765	GLN
1	D	770	HIS
1	E	762	GLN
1	G	762	GLN
1	G	765	GLN

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

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	ACT	B	903	-	1,3,3	1.16	0	0,3,3	0.00	-
3	PGE	E	901	-	9,9,9	0.32	0	8,8,8	0.36	0
2	SO4	B	901	-	4,4,4	0.18	0	6,6,6	0.18	0
3	PGE	B	902	-	9,9,9	0.31	0	8,8,8	0.42	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	E	901	-	-	3/7/7/7	-
3	PGE	B	902	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	901	PGE	O1-C1-C2-O2
3	B	902	PGE	O3-C5-C6-O4
3	E	901	PGE	O2-C3-C4-O3
3	E	901	PGE	O3-C5-C6-O4
3	B	902	PGE	C6-C5-O3-C4
3	B	902	PGE	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	903	ACT	3	0
3	B	902	PGE	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	78/81 (96%)	0.17	0 100 100	27, 37, 53, 58	0
1	B	78/81 (96%)	0.34	3 (3%) 40 41	28, 37, 56, 65	0
1	C	79/81 (97%)	0.46	1 (1%) 77 77	26, 46, 59, 71	0
1	D	75/81 (92%)	0.30	0 100 100	26, 41, 53, 64	0
1	E	79/81 (97%)	0.40	2 (2%) 57 58	31, 48, 60, 66	0
1	F	75/81 (92%)	0.25	1 (1%) 77 77	29, 42, 54, 59	0
1	G	78/81 (96%)	0.18	1 (1%) 77 77	27, 41, 53, 58	0
1	H	76/81 (93%)	0.27	4 (5%) 26 27	28, 43, 65, 74	0
All	All	618/648 (95%)	0.30	12 (1%) 66 67	26, 42, 57, 74	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	759	GLN	3.8
1	B	763	ARG	3.1
1	E	837	LYS	3.0
1	H	762	GLN	2.7
1	H	796	LEU	2.6
1	G	828[A]	CYS	2.4
1	C	827	ILE	2.4
1	F	775	LEU	2.4
1	H	764	TYR	2.4
1	H	767	LEU	2.3
1	E	831	LEU	2.1
1	B	765	GLN	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PGE	E	901	10/10	0.82	0.26	54,62,64,69	0
4	ACT	B	903	4/4	0.88	0.33	37,42,42,48	0
3	PGE	B	902	10/10	0.90	0.20	30,34,43,44	0
5	CL	D	901	1/1	0.90	0.10	57,57,57,57	0
2	SO4	B	901	5/5	0.99	0.08	36,37,41,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.