



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 11:19 AM UTC

PDB ID : 5LXO / pdb_00005lxo
Title : Coiled-coil protein
Authors : Thiagarajan, 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 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

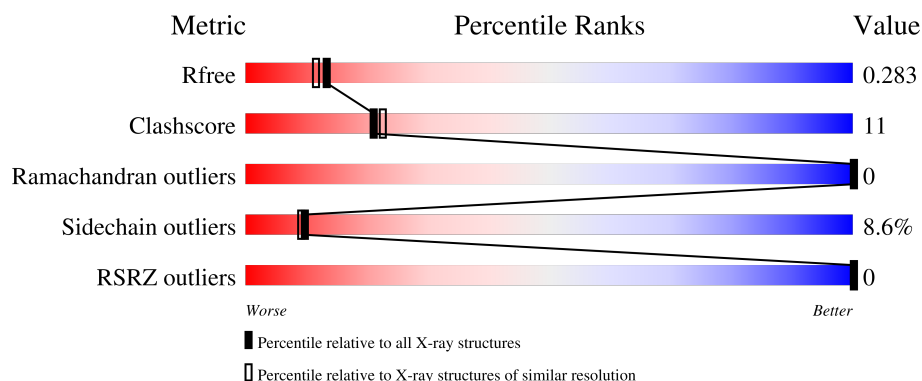
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (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 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	81	
1	B	81	
1	C	81	
1	D	81	
1	E	81	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	81	
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.

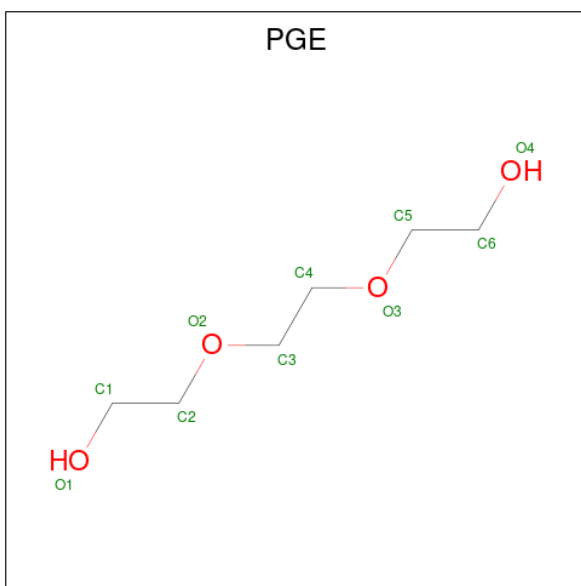
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	S	Se	0	1	0
			651	396	119	132	1	3			
1	B	80	Total	C	N	O	S	Se	0	3	0
			658	404	119	130	2	3			
1	C	81	Total	C	N	O	S	Se	0	3	0
			677	413	123	137	1	3			
1	D	77	Total	C	N	O	S	Se	0	3	0
			635	387	115	129	1	3			
1	E	81	Total	C	N	O	S	Se	0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

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



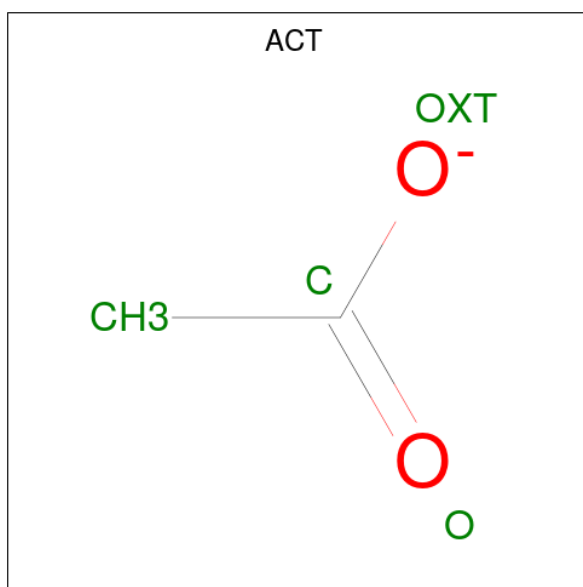
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: 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 (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is water.

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

Continued on next page...

Continued from previous page...

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, 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: Transforming acidic coiled-coil-containing protein 3

Chain A:  86% 12% .



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

Chain B:  67% 30% ..



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

Chain C:  73% 26% .



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

Chain D:  57% 30% 9% 5%



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

Chain E:  69% 26% 5%

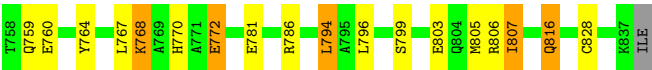
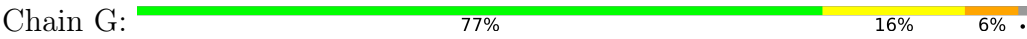


- Molecule 1: Transforming acidic coiled-coil-containing protein 3

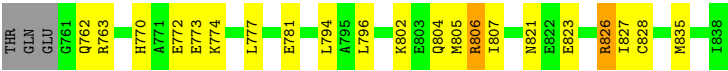
Chain F:  68% 23% . 5%



- 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)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.233 , 0.285 (Not available) , 0.283	Depositor DCC
R_{free} test set	1774 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	1.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.168 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5627	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, PGE, 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	0.53	0/650	0.77	0/861
1	B	0.51	0/666	0.82	1/881 (0.1%)
1	C	0.47	0/676	0.82	0/895
1	D	0.44	0/640	0.72	0/848
1	E	0.44	0/677	0.86	1/897 (0.1%)
1	F	0.46	0/625	0.71	0/828
1	G	0.56	0/648	0.88	2/859 (0.2%)
1	H	0.40	0/656	0.79	0/868
All	All	0.48	0/5238	0.80	4/6937 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	794	LEU	N-CA-C	8.95	120.64	111.07
1	G	816	GLN	N-CA-C	6.93	119.43	111.11
1	B	821	ASN	N-CA-C	5.33	118.00	111.82
1	E	761	GLY	N-CA-C	-5.10	108.34	114.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	651	0	667	8	0
1	B	658	0	690	18	0
1	C	677	0	695	17	0
1	D	635	0	652	27	1
1	E	672	0	698	23	0
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	4	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	117	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 (117) 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:HE21	1:E:762:GLN:HA	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:828:CYS:SG	6:B:1027:HOH:O	2.51	0.67
1:E:762:GLN:HA	1:E:762:GLN:NE2	1.96	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:E:768:LYS:NZ	6:E:1003:HOH:O	2.26	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:C:774:LYS:NZ	6:C:904:HOH:O	2.33	0.62
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: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:E:828:CYS:HB3	1:H:802:LYS:NZ	2.18	0.58
1:G:796:LEU:HD23	1:H:796:LEU:HB3	1.86	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:HE21	1:E:762:GLN:CA	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:815:GLU:O	1:D:818:THR:OG1	2.15	0.50
1:D:821:ASN:ND2	6:D:1006:HOH:O	2.38	0.50
1:A:819:LYS:NZ	6:A:904:HOH:O	2.43	0.49
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:HA	1:E:819:LYS:HD2	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:HE3	1:H:835[A]:MSE:HB3	1.78	0.43
1:C:781:GLU:O	1:C:785:VAL:HG13	2.19	0.43
1:F:834:LYS:NZ	6:F:907:HOH:O	2.42	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:760:GLU:O	1:C:761:GLY:C	2.63	0.41
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:HD2	1:F:819:LYS:HA	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:F:824:LEU:HD13	1:H:805[A]:MSE:HE1	2.03	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

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
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 ⓘ

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%)	68 (97%)	2 (3%)	37	47
1	B	72/68 (106%)	63 (88%)	9 (12%)	4	3
1	C	73/68 (107%)	71 (97%)	2 (3%)	39	50
1	D	69/68 (102%)	58 (84%)	11 (16%)	2	2
1	E	73/68 (107%)	66 (90%)	7 (10%)	8	7
1	F	67/68 (98%)	61 (91%)	6 (9%)	9	8
1	G	70/68 (103%)	63 (90%)	7 (10%)	7	6
1	H	71/68 (104%)	66 (93%)	5 (7%)	14	14
All	All	565/544 (104%)	516 (91%)	49 (9%)	10	9

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	790	GLN
1	A	812	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	763	ARG
1	B	773	GLU
1	B	774	LYS
1	B	782	ILE
1	B	790	GLN
1	B	808	GLN
1	B	822	GLU
1	B	828[A]	CYS
1	B	828[B]	CYS
1	C	765	GLN
1	C	822	GLU
1	D	760	GLU
1	D	772	GLU
1	D	774	LYS
1	D	776	GLN
1	D	786	ARG
1	D	800	LEU
1	D	812	LYS
1	D	825	THR
1	D	826	ARG
1	D	834	LYS
1	D	836	GLU
1	E	760	GLU
1	E	762	GLN
1	E	775	LEU
1	E	782	ILE
1	E	794	LEU
1	E	808	GLN
1	E	819	LYS
1	F	784	GLN
1	F	802	LYS
1	F	803	GLU
1	F	805[A]	MSE
1	F	805[B]	MSE
1	F	832	ILE
1	G	759	GLN
1	G	768	LYS
1	G	772	GLU
1	G	781	GLU
1	G	794	LEU
1	G	807	ILE
1	G	816	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	762	GLN
1	H	772	GLU
1	H	804	GLN
1	H	806	ARG
1	H	826	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	765	GLN
1	B	790	GLN
1	B	797	GLN
1	D	770	HIS
1	D	790	GLN
1	D	808	GLN
1	E	762	GLN
1	F	776	GLN
1	F	821	ASN
1	G	762	GLN
1	G	765	GLN
1	G	784	GLN
1	G	816	GLN
1	H	821	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	PGE	E	901	-	9,9,9	0.33	0	8,8,8	0.35	0
4	ACT	B	903	-	3,3,3	0.79	0	3,3,3	1.47	0
3	PGE	B	902	-	9,9,9	0.32	0	8,8,8	0.42	0
2	SO4	B	901	-	4,4,4	0.22	0	6,6,6	0.20	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	B	902	PGE	O3-C5-C6-O4
3	E	901	PGE	O1-C1-C2-O2
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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%)	-1.24	0 100 100	27, 37, 53, 58	0
1	B	78/81 (96%)	-1.22	0 100 100	21, 37, 56, 65	2 (2%)
1	C	79/81 (97%)	-1.12	0 100 100	18, 45, 59, 71	2 (2%)
1	D	75/81 (92%)	-1.15	0 100 100	19, 41, 53, 64	2 (2%)
1	E	79/81 (97%)	-1.14	0 100 100	24, 47, 60, 66	3 (3%)
1	F	75/81 (92%)	-1.19	0 100 100	29, 42, 54, 59	0
1	G	78/81 (96%)	-1.19	0 100 100	21, 41, 53, 58	1 (1%)
1	H	76/81 (93%)	-1.18	0 100 100	20, 43, 65, 74	2 (2%)
All	All	618/648 (95%)	-1.18	0 100 100	18, 41, 57, 74	12 (1%)

There are no RSRZ outliers to report.

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($\text{\AA}^2$)	Q<0.9
3	PGE	E	901	10/10	0.96	0.06	54,62,64,69	0
3	PGE	B	902	10/10	0.98	0.04	30,34,43,44	0
4	ACT	B	903	4/4	0.98	0.09	37,42,42,48	0
2	SO4	B	901	5/5	0.99	0.03	36,37,41,44	0
5	CL	D	901	1/1	0.99	0.06	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.