



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 07:09 PM EDT

PDB ID : 5LXN  
Title : Coiled-coil protein  
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Deposited on : 2016-09-22  
Resolution : 2.08 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](mailto: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>.

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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	:	2.37.1
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)	:	2.37.1

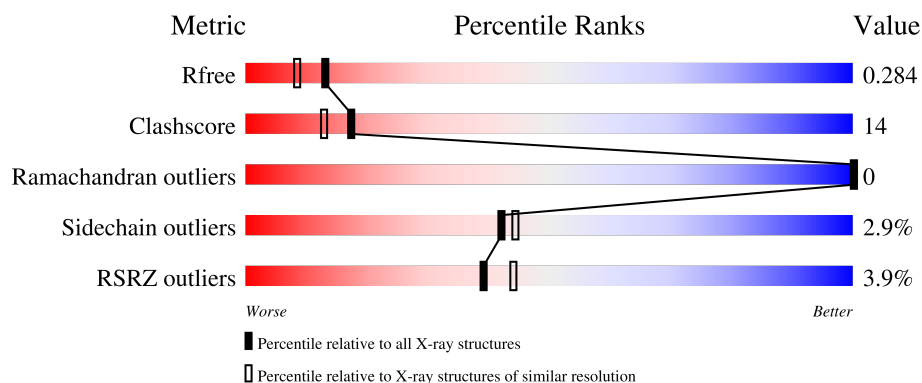
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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  $\geq 3$ , 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	<div> <div>2%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
1	B	81	<div> <div>10%</div> <div>64%</div> <div>35%</div> <div>.</div> </div>
1	C	81	<div> <div>4%</div> <div>62%</div> <div>36%</div> <div>.</div> </div>
1	D	81	<div> <div>4%</div> <div>68%</div> <div>31%</div> <div>.</div> </div>
1	E	81	<div> <div>5%</div> <div>72%</div> <div>27%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	81	 % 72% 21% 6%
1	G	81	 % 77% 22%
1	H	81	 2% 73% 26%

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
2	PGE	A	901	-	-	-	X
2	PGE	G	901	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5817 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	81	Total	C	N	O	S	Se	0	3	0
			667	410	119	134	1	3			
1	B	80	Total	C	N	O	S	Se	0	3	0
			663	405	120	132	2	4			
1	C	81	Total	C	N	O	S	Se	0	5	0
			689	422	125	138	1	3			
1	D	80	Total	C	N	O	S	Se	0	2	0
			656	400	120	133	1	2			
1	E	81	Total	C	N	O	S	Se	0	0	0
			651	397	119	132	1	2			
1	F	76	Total	C	N	O	S	Se	0	1	0
			617	376	113	124	1	3			
1	G	80	Total	C	N	O	S	Se	0	0	0
			643	391	118	131	1	2			
1	H	80	Total	C	N	O	S	Se	0	6	0
			690	421	128	136	2	3			

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			10	6	4		
2	G	1	Total	C	O	0	0
			10	6	4		
2	G	1	Total	C	O	0	0
			10	6	4		
2	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

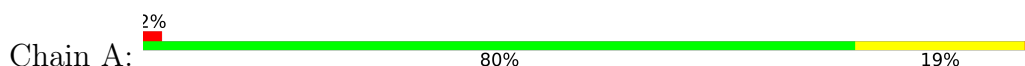
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		
4	B	49	Total	O	0	0
			49	49		
4	C	56	Total	O	0	0
			56	56		
4	D	60	Total	O	0	0
			60	60		
4	E	53	Total	O	0	0
			53	53		
4	F	53	Total	O	0	0
			53	53		
4	G	64	Total	O	0	0
			64	64		
4	H	62	Total	O	0	0
			62	62		

### 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



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



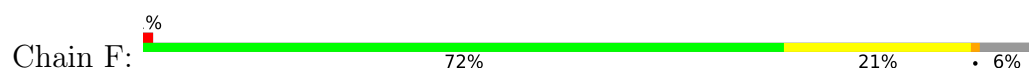
- Molecule 1: Transforming acidic coiled-coil-containing protein 3



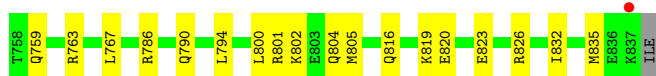
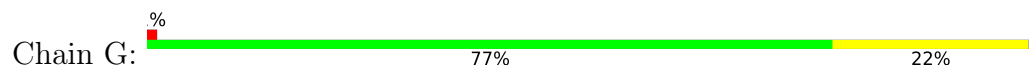
- Molecule 1: Transforming acidic coiled-coil-containing protein 3



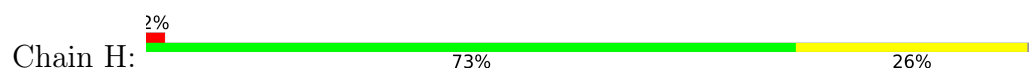
- Molecule 1: Transforming acidic coiled-coil-containing protein 3



- 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, $\alpha$ , $\beta$ , $\gamma$	57.39Å 76.78Å 86.83Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	28.76 – 2.08 28.76 – 2.08	Depositor EDS
% Data completeness (in resolution range)	82.6 (28.76-2.08) 82.2 (28.76-2.08)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.227 , 0.285 0.231 , 0.284	Depositor DCC
$R_{free}$ test set	1897 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	1.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 28.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.166 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5817	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PGE, SO4

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	0.27	0/675	0.44	0/895
1	B	0.28	0/665	0.50	0/880
1	C	0.33	0/694	0.45	0/918
1	D	0.21	0/658	0.45	0/872
1	E	0.25	0/650	0.43	0/862
1	F	0.24	0/616	0.41	0/816
1	G	0.21	0/642	0.39	0/851
1	H	0.27	0/694	0.43	0/916
All	All	0.26	0/5294	0.44	0/7010

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	667	0	696	18	0
1	B	663	0	684	30	0
1	C	689	0	716	43	2
1	D	656	0	675	35	2
1	E	651	0	671	16	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	617	0	634	16	0
1	G	643	0	660	16	1
1	H	690	0	718	17	1
2	A	20	0	28	2	0
2	B	10	0	14	1	0
2	D	10	0	14	4	0
2	G	20	0	28	6	0
2	H	10	0	14	1	0
3	D	10	0	0	0	0
4	A	64	0	0	2	0
4	B	49	0	0	4	1
4	C	56	0	0	8	0
4	D	60	0	0	5	0
4	E	53	0	0	2	2
4	F	53	0	0	3	0
4	G	64	0	0	0	0
4	H	62	0	0	3	0
All	All	5817	0	5552	149	5

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 14.

All (149) 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:C:763:ARG:NE	1:D:760:GLU:OE2	1.63	1.28
1:C:763:ARG:HH21	1:D:760:GLU:CD	1.43	1.21
1:A:802:LYS:NZ	4:A:1002:HOH:O	1.75	1.17
1:C:763:ARG:CZ	1:D:760:GLU:OE2	1.93	1.15
1:C:763:ARG:NH2	1:D:760:GLU:OE2	1.83	1.09
1:D:760:GLU:HB2	4:D:1011:HOH:O	1.59	0.99
1:D:760:GLU:CB	4:D:1011:HOH:O	2.10	0.97
1:B:815:GLU:OE1	4:B:1001:HOH:O	1.84	0.94
1:C:763:ARG:NH2	1:D:760:GLU:CD	2.18	0.93
1:A:836:GLU:OE1	4:A:1003:HOH:O	1.94	0.85
1:C:804:GLN:HE21	1:C:808:GLN:HE21	1.28	0.79
1:B:812:LYS:HA	1:B:815:GLU:HG2	1.67	0.76
1:E:768:LYS:NZ	4:E:901:HOH:O	2.14	0.76
1:E:786:ARG:HG2	1:E:790:GLN:HE21	1.51	0.74
1:B:806:ARG:NH2	4:B:1002:HOH:O	2.12	0.74
1:C:763:ARG:NH2	1:D:760:GLU:OE1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:817:LYS:O	1:F:821:ASN:ND2	2.22	0.72
1:E:828:CYS:HB2	1:F:828:CYS:SG	2.28	0.71
1:C:779:ASN:HA	1:C:782:ILE:HD12	1.70	0.71
1:D:760:GLU:HG2	1:D:764:TYR:CD2	2.25	0.71
1:E:768:LYS:HG3	1:F:767:LEU:HD21	1.72	0.71
1:E:821:ASN:ND2	4:F:901:HOH:O	2.25	0.69
1:A:796[B]:LEU:HD11	1:B:796:LEU:HB3	1.73	0.68
1:C:823[A]:GLU:OE1	4:C:901:HOH:O	2.12	0.68
1:G:820:GLU:HG3	2:G:901:PGE:H5	1.76	0.67
1:A:832:ILE:HG23	1:F:795:ALA:HB1	1.77	0.67
1:C:821:ASN:OD1	1:D:821:ASN:ND2	2.28	0.66
1:C:762[A]:GLN:NE2	4:C:904:HOH:O	2.28	0.62
1:D:827:ILE:HD13	1:H:801:ARG:HE	1.64	0.62
1:F:784:GLN:O	1:G:759:GLN:NE2	2.26	0.62
1:D:827:ILE:CD1	1:H:801:ARG:HB3	2.29	0.62
1:D:827:ILE:HD12	1:H:801:ARG:HB3	1.82	0.61
1:B:763:ARG:O	1:B:766:ALA:HB3	2.01	0.61
1:C:812[B]:LYS:NZ	4:C:906:HOH:O	2.33	0.61
1:C:822:GLU:OE2	4:C:902:HOH:O	2.16	0.60
1:A:835:MSE:HG3	1:B:835[B]:MSE:HE2	1.82	0.60
1:G:819:LYS:NZ	2:G:901:PGE:O4	2.35	0.59
1:E:827:ILE:O	1:E:830:ASP:OD1	2.21	0.58
1:D:810:LEU:HG	2:D:901:PGE:H6	1.86	0.58
1:D:760:GLU:CG	4:D:1011:HOH:O	2.47	0.58
1:C:811:GLU:HG2	2:D:901:PGE:H32	1.87	0.57
1:C:782:ILE:HA	1:D:782:ILE:HD13	1.86	0.57
1:C:835[A]:MSE:HE3	1:H:791:ALA:HA	1.85	0.57
1:D:826:ARG:NH1	4:D:1005:HOH:O	2.37	0.57
1:H:774:LYS:NZ	4:H:1004:HOH:O	2.36	0.57
1:C:819:LYS:NZ	4:C:903:HOH:O	2.28	0.56
1:B:763:ARG:O	1:B:767:LEU:HD12	2.06	0.56
1:G:816:GLN:HB2	2:G:901:PGE:H12	1.88	0.56
1:F:820:GLU:OE1	4:F:901:HOH:O	2.18	0.56
1:C:806:ARG:NH2	4:C:909:HOH:O	2.38	0.55
1:D:776[B]:GLN:OE1	1:D:777:LEU:N	2.40	0.55
1:C:785:VAL:HG21	1:D:782:ILE:HD11	1.88	0.55
1:G:816:GLN:HA	2:G:901:PGE:H42	1.89	0.55
1:F:819:LYS:O	1:F:822:GLU:HG2	2.05	0.55
1:H:831:LEU:HD11	1:H:835:MSE:HE3	1.89	0.55
1:D:760:GLU:CG	1:D:764:TYR:CD2	2.91	0.54
1:E:825:THR:O	1:E:825:THR:HG22	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:MSE:HG3	1:B:835[A]:MSE:HE3	1.90	0.54
1:A:835:MSE:HE3	1:B:835[A]:MSE:SE	2.57	0.54
1:A:836:GLU:HG2	1:A:837:LYS:CG	2.39	0.53
1:C:819:LYS:HE3	4:C:901:HOH:O	2.08	0.53
1:A:815:GLU:HG3	2:A:901:PGE:H32	1.91	0.52
1:G:823:GLU:HG2	1:G:826:ARG:HH22	1.75	0.52
1:C:774:LYS:NZ	4:C:905:HOH:O	2.31	0.51
1:F:792:GLU:OE2	4:F:902:HOH:O	2.18	0.51
1:B:832:ILE:HG23	1:G:767:LEU:HD22	1.92	0.51
1:C:765:GLN:HA	1:C:768:LYS:HB3	1.91	0.51
1:H:776:GLN:NE2	1:H:780:GLU:OE2	2.43	0.51
1:C:822:GLU:N	1:C:822:GLU:OE1	2.43	0.51
1:A:801:ARG:CZ	1:D:826:ARG:HH21	2.24	0.51
1:B:801:ARG:NH2	4:B:1010:HOH:O	2.44	0.50
1:C:825:THR:HG22	1:D:824:LEU:HD11	1.94	0.50
1:B:831:LEU:HD11	1:B:835[B]:MSE:HE3	1.94	0.50
1:H:797:GLN:HG2	4:H:1039:HOH:O	2.11	0.50
1:C:831:LEU:HD21	1:D:831:LEU:HD22	1.92	0.50
1:B:823:GLU:OE2	4:B:1003:HOH:O	2.20	0.49
1:C:821:ASN:HB2	1:C:822:GLU:OE1	2.13	0.49
1:G:835:MSE:HG3	1:H:835:MSE:HE2	1.94	0.49
1:E:780:GLU:O	1:E:784:GLN:HB2	2.13	0.49
1:F:776:GLN:O	1:F:780:GLU:HG3	2.12	0.49
1:E:764:TYR:OH	4:E:902:HOH:O	2.15	0.49
1:G:800:LEU:O	1:G:804:GLN:HG3	2.13	0.48
1:A:759:GLN:O	1:A:763:ARG:HG3	2.13	0.48
1:G:819:LYS:HB3	2:G:901:PGE:H4	1.94	0.48
1:B:812:LYS:HA	1:B:815:GLU:CG	2.41	0.48
1:A:803:GLU:HA	1:A:803:GLU:OE1	2.14	0.48
1:B:791:ALA:HB1	1:E:835:MSE:O	2.13	0.48
1:C:781:GLU:OE2	1:D:786:ARG:NH2	2.45	0.48
1:G:759:GLN:O	1:G:763:ARG:HG3	2.14	0.47
1:D:795:ALA:HB1	1:G:832:ILE:HG23	1.96	0.47
1:C:821:ASN:ND2	4:D:1001:HOH:O	2.47	0.47
1:B:802:LYS:O	1:B:806:ARG:HG3	2.14	0.47
1:A:836:GLU:HG2	1:A:837:LYS:HG2	1.95	0.47
1:E:800:LEU:O	1:E:804:GLN:HG3	2.15	0.46
1:H:817:LYS:HZ3	2:H:901:PGE:H12	1.80	0.46
1:A:835:MSE:HG3	1:B:835[B]:MSE:CE	2.45	0.46
1:G:819:LYS:HG2	2:G:901:PGE:H52	1.97	0.46
1:C:819:LYS:HD2	1:C:819:LYS:HA	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:762:GLN:H	1:H:762:GLN:CD	2.13	0.46
1:H:829:ASP:OD1	4:H:1001:HOH:O	2.20	0.46
1:B:788:LYS:HG2	1:E:838:ILE:HG13	1.98	0.46
1:C:768:LYS:O	1:C:772:GLU:HB2	2.16	0.45
1:B:759:GLN:HG2	1:B:763:ARG:NH2	2.31	0.45
1:G:823:GLU:HG2	1:G:826:ARG:NH2	2.31	0.45
1:D:822:GLU:O	1:D:826:ARG:HG3	2.17	0.45
1:G:801:ARG:O	1:G:805:MSE:HG2	2.16	0.45
1:C:758:THR:HB	1:C:760:GLU:HG2	1.98	0.45
1:C:811:GLU:OE2	1:D:806:ARG:NH2	2.48	0.45
1:H:818:THR:O	1:H:822:GLU:HG3	2.17	0.44
1:A:836:GLU:HG2	1:A:837:LYS:HG3	1.99	0.44
1:C:838:ILE:O	1:H:788:LYS:HE2	2.17	0.44
1:E:786:ARG:HG2	1:E:790:GLN:NE2	2.25	0.44
1:E:779:ASN:HA	1:E:782:ILE:HG22	2.00	0.44
1:D:823:GLU:O	1:D:827:ILE:HG12	2.18	0.43
1:B:759:GLN:HG2	1:B:763:ARG:CZ	2.48	0.43
1:C:835[A]:MSE:HE2	1:H:794:LEU:HD12	2.01	0.43
1:F:777:LEU:HD23	1:F:780:GLU:OE1	2.19	0.43
1:C:811:GLU:HG2	2:D:901:PGE:H2	2.00	0.43
1:C:838:ILE:HD13	1:C:838:ILE:HA	1.81	0.43
1:C:830:ASP:O	1:C:834:LYS:HG3	2.19	0.43
1:H:800:LEU:O	1:H:804[B]:GLN:HG3	2.19	0.43
1:A:819:LYS:HD3	2:A:901:PGE:H4	1.99	0.43
1:B:770:HIS:NE2	1:B:774:LYS:HE3	2.34	0.43
1:C:765:GLN:OE1	1:C:765:GLN:N	2.52	0.43
1:E:832:ILE:O	1:E:836:GLU:HG2	2.19	0.43
1:F:780:GLU:O	1:F:784:GLN:HG3	2.19	0.43
1:A:800:LEU:O	1:A:804:GLN:HG3	2.19	0.42
1:C:806:ARG:HG3	1:D:807:ILE:HD12	2.02	0.42
1:B:764:TYR:C	1:B:766:ALA:N	2.72	0.42
1:C:817[B]:LYS:NZ	1:D:818:THR:OG1	2.53	0.42
1:D:806:ARG:HE	2:D:901:PGE:H5	1.84	0.42
1:B:805[B]:MSE:HG2	1:F:823:GLU:CD	2.40	0.42
1:B:799:SER:O	1:B:803:GLU:HG2	2.20	0.42
1:C:835[B]:MSE:HB2	1:H:795:ALA:HB2	2.02	0.41
1:E:788:LYS:HB2	1:E:788:LYS:HE2	1.72	0.41
1:F:775:LEU:HD23	1:F:775:LEU:HA	1.75	0.41
1:B:805[A]:MSE:HG3	1:B:806:ARG:N	2.35	0.41
1:B:813:THR:HG23	2:B:901:PGE:H42	2.03	0.41
1:B:827:ILE:HD12	1:F:805[A]:MSE:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:786:ARG:O	1:G:790:GLN:HG3	2.21	0.41
1:C:767:LEU:CD2	1:D:767:LEU:HD23	2.51	0.41
1:C:767:LEU:HD23	1:D:767:LEU:HD23	2.02	0.41
1:B:828[A]:CYS:O	1:B:832:ILE:HG13	2.21	0.40
1:A:788:LYS:HE3	1:A:788:LYS:HB2	1.84	0.40
1:B:812:LYS:CG	1:F:816:GLN:HE21	2.35	0.40
1:B:818:THR:O	1:B:822:GLU:HG3	2.21	0.40
1:D:781:GLU:O	1:D:785:VAL:HG23	2.21	0.40
1:F:775:LEU:HD23	1:F:778:ALA:HB3	2.03	0.40

All (5) 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:C:772:GLU:OE2	1:G:802:LYS:NZ[1_556]	2.12	0.08
1:E:788:LYS:NZ	1:H:837:LYS:O[2_555]	2.14	0.06
1:D:835:MSE:O	4:E:902:HOH:O[1_556]	2.15	0.05
1:C:763:ARG:NH1	4:B:1001:HOH:O[2_546]	2.17	0.03
1:D:833:SER:O	4:E:901:HOH:O[1_556]	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	82/81 (101%)	81 (99%)	1 (1%)	0	100	100
1	B	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
1	C	84/81 (104%)	84 (100%)	0	0	100	100
1	D	80/81 (99%)	79 (99%)	1 (1%)	0	100	100
1	E	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
1	F	75/81 (93%)	75 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
1	H	84/81 (104%)	82 (98%)	2 (2%)	0	100	100
All	All	643/648 (99%)	634 (99%)	9 (1%)	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	73/68 (107%)	70 (96%)	3 (4%)	30	30
1	B	72/68 (106%)	71 (99%)	1 (1%)	67	72
1	C	75/68 (110%)	71 (95%)	4 (5%)	22	20
1	D	71/68 (104%)	70 (99%)	1 (1%)	67	72
1	E	70/68 (103%)	66 (94%)	4 (6%)	20	17
1	F	66/68 (97%)	65 (98%)	1 (2%)	65	69
1	G	69/68 (102%)	68 (99%)	1 (1%)	67	72
1	H	75/68 (110%)	72 (96%)	3 (4%)	31	31
All	All	571/544 (105%)	553 (97%)	18 (3%)	42	40

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	803	GLU
1	A	805[A]	MSE
1	A	805[B]	MSE
1	B	784	GLN
1	C	758	THR
1	C	759	GLN
1	C	774	LYS
1	C	828	CYS
1	D	773	GLU

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Mol	Chain	Res	Type
1	E	772	GLU
1	E	826	ARG
1	E	828	CYS
1	E	829	ASP
1	F	775	LEU
1	G	794	LEU
1	H	805[A]	MSE
1	H	805[B]	MSE
1	H	838	ILE

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

Mol	Chain	Res	Type
1	C	808	GLN
1	E	762	GLN
1	E	790	GLN
1	F	816	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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	$\# Z  > 2$
2	PGE	A	902	-	9,9,9	0.30	0	8,8,8	0.28	0
2	PGE	D	901	-	9,9,9	0.30	0	8,8,8	0.28	0
2	PGE	G	902	-	9,9,9	0.30	0	8,8,8	0.30	0
3	SO4	D	903	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	D	902	-	4,4,4	0.16	0	6,6,6	0.04	0
2	PGE	G	901	-	9,9,9	0.29	0	8,8,8	0.33	0
2	PGE	A	901	-	9,9,9	0.30	0	8,8,8	0.29	0
2	PGE	H	901	-	9,9,9	0.31	0	8,8,8	0.29	0
2	PGE	B	901	-	9,9,9	0.31	0	8,8,8	0.27	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
2	PGE	A	902	-	-	3/7/7/7	-
2	PGE	D	901	-	-	1/7/7/7	-
2	PGE	G	902	-	-	3/7/7/7	-
2	PGE	G	901	-	-	3/7/7/7	-
2	PGE	A	901	-	-	3/7/7/7	-
2	PGE	H	901	-	-	4/7/7/7	-
2	PGE	B	901	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	PGE	O2-C3-C4-O3
2	H	901	PGE	O2-C3-C4-O3
2	G	902	PGE	O1-C1-C2-O2
2	A	902	PGE	O2-C3-C4-O3
2	G	902	PGE	O2-C3-C4-O3
2	A	902	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
2	G	902	PGE	O3-C5-C6-O4
2	H	901	PGE	C1-C2-O2-C3
2	D	901	PGE	O1-C1-C2-O2
2	H	901	PGE	C3-C4-O3-C5
2	G	901	PGE	O2-C3-C4-O3
2	G	901	PGE	C4-C3-O2-C2
2	A	902	PGE	C1-C2-O2-C3
2	H	901	PGE	C4-C3-O2-C2
2	B	901	PGE	C3-C4-O3-C5
2	G	901	PGE	C1-C2-O2-C3
2	A	901	PGE	C4-C3-O2-C2
2	A	901	PGE	C3-C4-O3-C5

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	901	PGE	4	0
2	G	901	PGE	6	0
2	A	901	PGE	2	0
2	H	901	PGE	1	0
2	B	901	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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	79/81 (97%)	0.44	2 (2%) 57 62	26, 43, 59, 68	0
1	B	78/81 (96%)	0.59	8 (10%) 6 8	29, 49, 74, 81	0
1	C	79/81 (97%)	0.61	3 (3%) 40 45	29, 49, 61, 70	0
1	D	78/81 (96%)	0.61	3 (3%) 40 45	27, 43, 61, 65	0
1	E	79/81 (97%)	0.56	4 (5%) 28 32	25, 49, 65, 77	0
1	F	74/81 (91%)	0.45	1 (1%) 75 78	28, 46, 59, 65	0
1	G	78/81 (96%)	0.25	1 (1%) 77 79	28, 39, 55, 67	0
1	H	78/81 (96%)	0.51	2 (2%) 56 60	27, 39, 65, 84	0
All	All	623/648 (96%)	0.50	24 (3%) 39 44	25, 45, 63, 84	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	759	GLN	6.3
1	D	838	ILE	5.9
1	C	758	THR	4.7
1	D	760	GLU	4.3
1	H	838	ILE	3.9
1	E	838	ILE	3.9
1	E	827	ILE	3.8
1	B	759	GLN	3.3
1	C	764	TYR	3.2
1	B	762	GLN	2.9
1	B	764	TYR	2.8
1	E	758	THR	2.6
1	G	837	LYS	2.6
1	B	761	GLY	2.6
1	C	765	GLN	2.5
1	F	775	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	759	GLN	2.4
1	B	793	ALA	2.3
1	A	838	ILE	2.2
1	E	837	LYS	2.2
1	A	786	ARG	2.1
1	B	795	ALA	2.1
1	B	766	ALA	2.0
1	B	804	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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PGE	A	901	10/10	0.62	0.50	39,57,76,76	0
2	PGE	G	901	10/10	0.75	0.27	37,53,59,68	0
2	PGE	H	901	10/10	0.81	0.25	36,48,61,64	0
2	PGE	A	902	10/10	0.82	0.33	28,41,55,60	0
2	PGE	G	902	10/10	0.83	0.38	28,50,56,58	0
2	PGE	D	901	10/10	0.86	0.36	28,48,57,60	0
2	PGE	B	901	10/10	0.90	0.19	32,42,45,46	0
3	SO4	D	903	5/5	0.90	0.14	48,57,71,74	0
3	SO4	D	902	5/5	0.98	0.09	39,40,51,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.