



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2018 – 12:39 AM EST

PDB ID : 5ODS
Title : Structure of a phosphoprotein-protein complex
Authors : Mukherjee, M.; Bayliss, R.
Deposited on : 2017-07-06
Resolution : 3.09 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

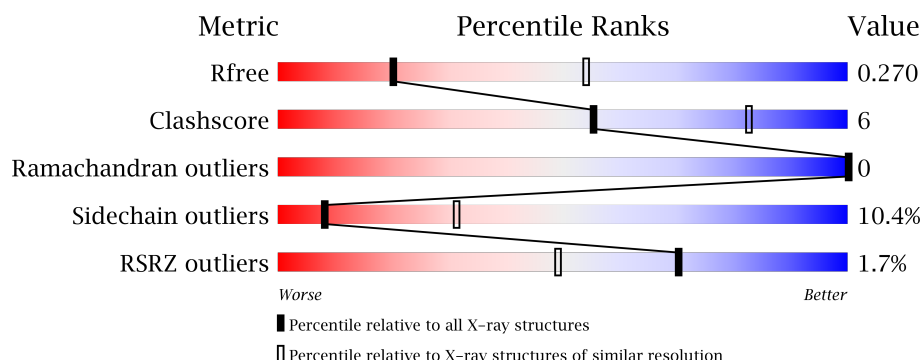
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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. 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	574	
1	B	574	
1	C	574	
1	D	574	
2	E	18	

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Mol	Chain	Length	Quality of chain
2	F	18	<div><div></div><div>6%</div><div>83%</div><div>11%</div><div>6%</div></div>
2	G	18	<div><div></div><div>6%</div><div>83%</div><div>17%</div><div></div></div>
2	H	18	<div><div></div><div>6%</div><div>72%</div><div>22%</div><div>6%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18224 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 Clathrin heavy chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4474	2854	761	834	25			
1	B	567	Total	C	N	O	S	0	0	0
			4417	2823	748	821	25			
1	C	554	Total	C	N	O	S	0	0	0
			4321	2764	735	797	25			
1	D	571	Total	C	N	O	S	0	0	0
			4432	2831	751	825	25			

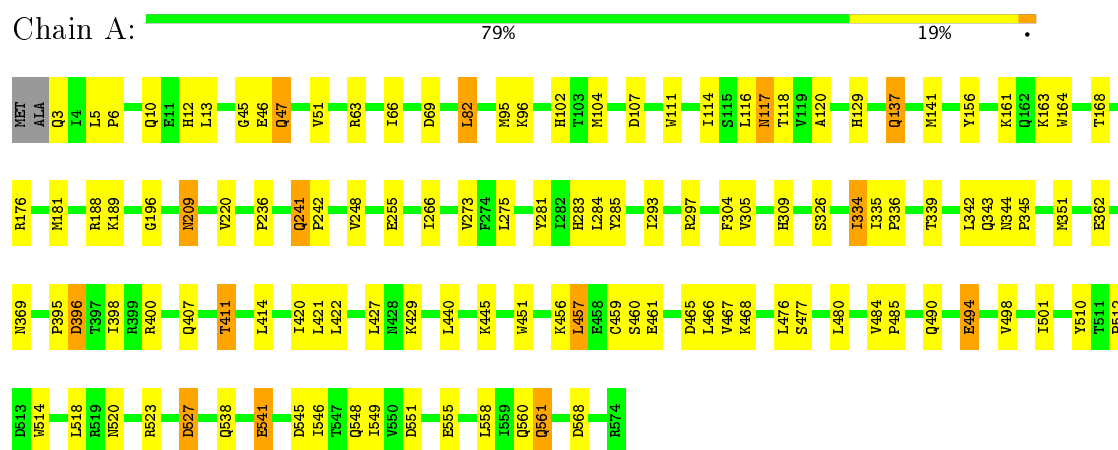
- Molecule 2 is a protein called LYS-GLU-SER-ALA-LEU-ARG-LYS-GLN-SEP-LEU-TYR-LEU-LYS-PHE-ASP-PRO-LEU-LEU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			147	95	24	27	1			
2	F	18	Total	C	N	O	P	0	0	0
			143	92	23	27	1			
2	G	18	Total	C	N	O	P	0	0	0
			143	92	23	27	1			
2	H	18	Total	C	N	O	P	0	0	0
			147	95	24	27	1			

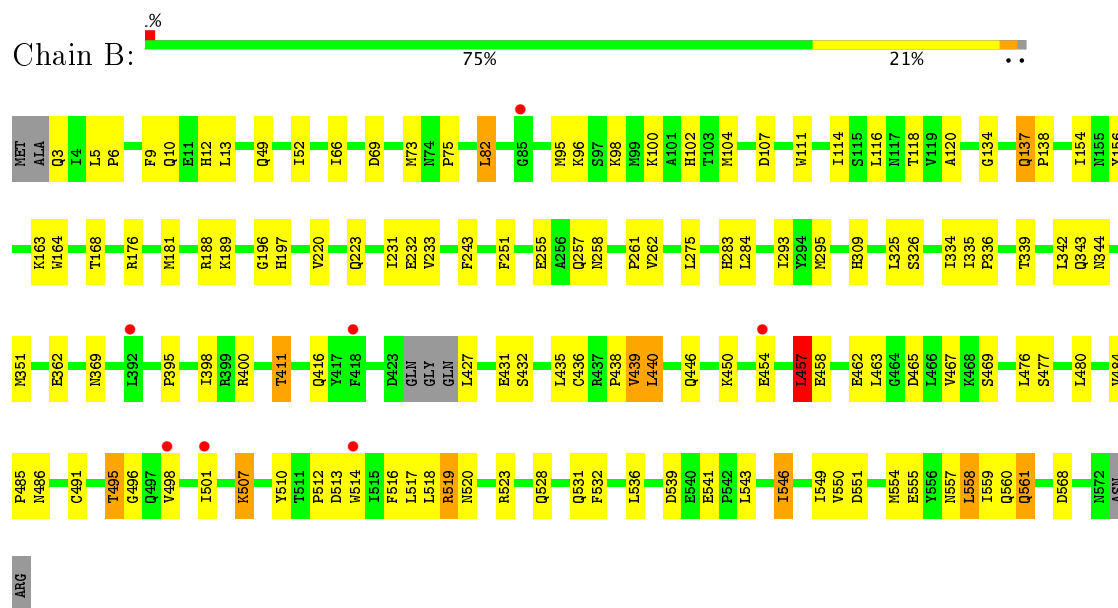
3 Residue-property plots

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.

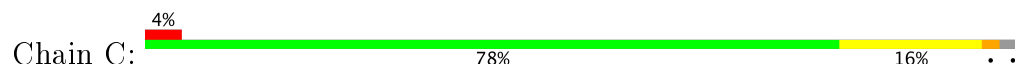
• Molecule 1: Clathrin heavy chain 1

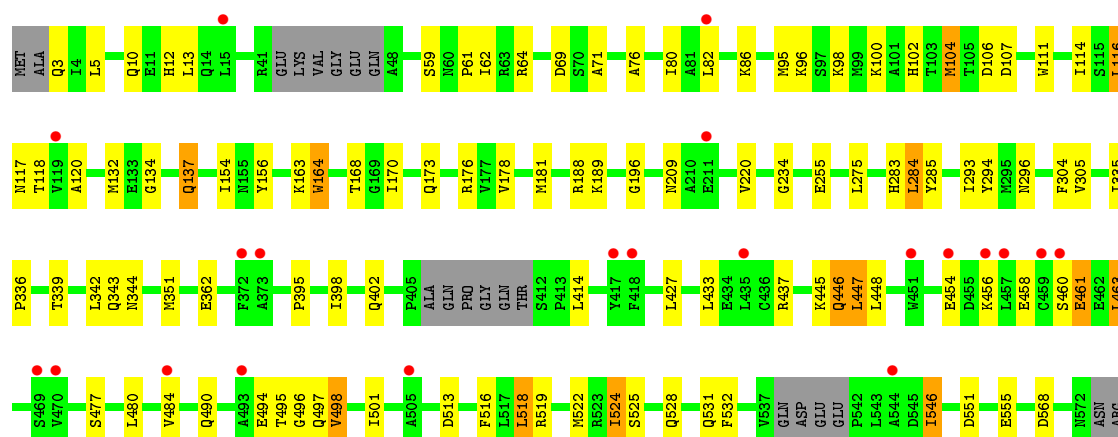


• Molecule 1: Clathrin heavy chain 1

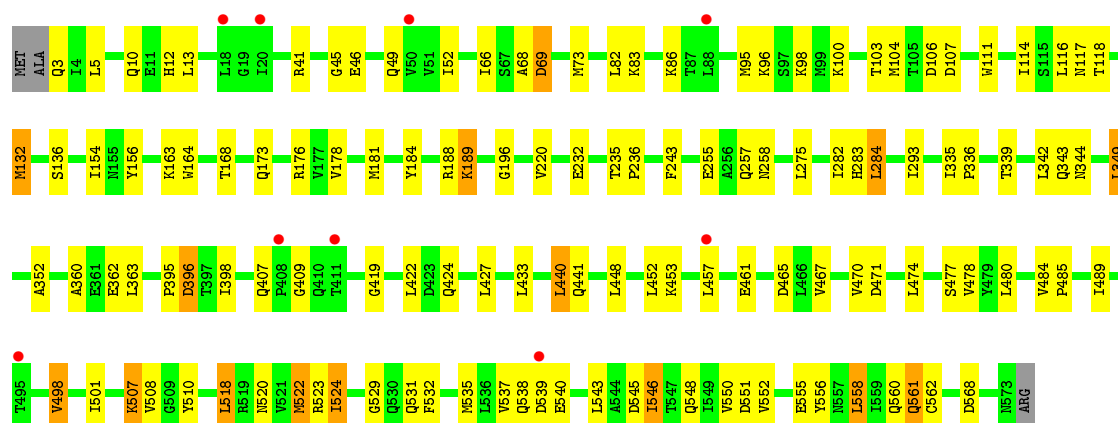
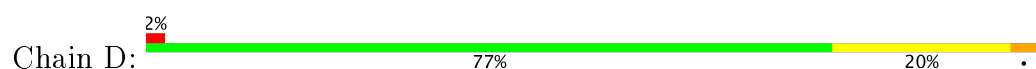


• Molecule 1: Clathrin heavy chain 1

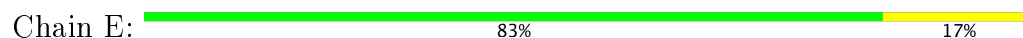




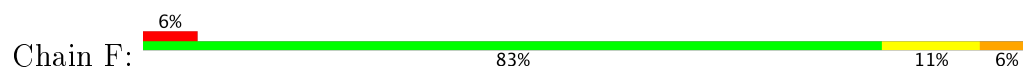
• Molecule 1: Clathrin heavy chain 1



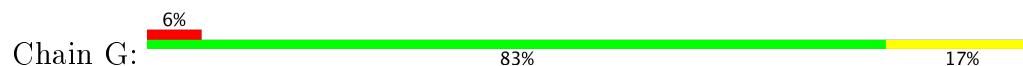
• Molecule 2: LYS-GLU-SER-ALA-LEU-ARG-LYS-GLN-SEP-LEU-TYR-LEU-LYS-PHE-ASP-PRO-LEU-LEU

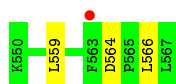


• Molecule 2: LYS-GLU-SER-ALA-LEU-ARG-LYS-GLN-SEP-LEU-TYR-LEU-LYS-PHE-ASP-PRO-LEU-LEU



• Molecule 2: LYS-GLU-SER-ALA-LEU-ARG-LYS-GLN-SEP-LEU-TYR-LEU-LYS-PHE-ASP-PRO-LEU-LEU





- Molecule 2: LYS-GLU-SER-ALA-LEU-ARG-LYS-GLN-SEP-LEU-TYR-LEU-LYS-PHE-ASP-PRO-LEU-LEU

Chain H:
6% 72% 22% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.52Å 120.04Å 123.13Å 90.00° 95.72° 90.00°	Depositor
Resolution (Å)	61.26 – 3.09 61.26 – 3.09	Depositor EDS
% Data completeness (in resolution range)	98.7 (61.26-3.09) 98.7 (61.26-3.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.221 , 0.269 0.222 , 0.270	Depositor DCC
R_{free} test set	2886 reflections (4.76%)	DCC
Wilson B-factor (Å ²)	99.4	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 84.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18224	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: SEP

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	0.29	0/4564	0.59	2/6194 (0.0%)
1	B	0.31	0/4506	0.59	2/6118 (0.0%)
1	C	0.29	0/4405	0.57	0/5974
1	D	0.32	0/4522	0.62	1/6143 (0.0%)
2	E	0.23	0/138	0.54	0/183
2	F	0.28	0/134	0.60	0/179
2	G	0.23	0/134	0.54	0/179
2	H	0.24	0/138	0.43	0/183
All	All	0.30	0/18541	0.59	5/25153 (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	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	241	GLN	C-N-CD	-7.09	105.01	120.60
1	B	457	LEU	CA-CB-CG	6.73	130.78	115.30
1	D	556	TYR	N-CA-C	6.11	127.49	111.00
1	B	440	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	241	GLN	C-N-CA	5.31	144.29	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4474	0	4479	50	0
1	B	4417	0	4411	60	0
1	C	4321	0	4336	47	0
1	D	4432	0	4414	60	0
2	E	147	0	148	1	0
2	F	143	0	137	2	0
2	G	143	0	137	1	0
2	H	147	0	148	4	0
All	All	18224	0	18210	216	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 216 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:460:SER:H	1:C:463:LEU:HD11	1.43	0.82
1:D:537:VAL:HG23	1:D:538:GLN:HG2	1.65	0.78
1:D:275:LEU:HB3	1:D:283:HIS:HB2	1.69	0.74
1:B:275:LEU:HB3	1:B:283:HIS:HB2	1.69	0.73
1:C:494:GLU:HA	1:C:524:ILE:HG21	1.70	0.73

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	570/574 (99%)	545 (96%)	25 (4%)	0	100	100
1	B	563/574 (98%)	532 (94%)	31 (6%)	0	100	100
1	C	544/574 (95%)	518 (95%)	26 (5%)	0	100	100
1	D	569/574 (99%)	538 (95%)	31 (5%)	0	100	100
2	E	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
2	F	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
2	G	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
2	H	15/18 (83%)	15 (100%)	0	0	100	100
All	All	2306/2368 (97%)	2190 (95%)	116 (5%)	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	486/494 (98%)	433 (89%)	53 (11%)	7	30
1	B	477/494 (97%)	427 (90%)	50 (10%)	8	31
1	C	469/494 (95%)	426 (91%)	43 (9%)	11	39
1	D	477/494 (97%)	428 (90%)	49 (10%)	8	32
2	E	14/16 (88%)	12 (86%)	2 (14%)	4	17
2	F	13/16 (81%)	11 (85%)	2 (15%)	3	14
2	G	13/16 (81%)	11 (85%)	2 (15%)	3	14
2	H	14/16 (88%)	11 (79%)	3 (21%)	1	5
All	All	1963/2040 (96%)	1759 (90%)	204 (10%)	8	31

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	519	ARG
1	C	116	LEU
1	D	522	MET
1	B	539	ASP
1	C	3	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	309	HIS
1	B	528	GLN
1	D	17	ASN
1	B	102	HIS
1	C	102	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	SEP	E	558	2	9,9,10	1.40	1 (11%)	9,12,14	2.04	2 (22%)
2	SEP	F	558	2	9,9,10	1.38	1 (11%)	9,12,14	2.00	2 (22%)
2	SEP	G	558	2	9,9,10	1.40	1 (11%)	9,12,14	2.05	2 (22%)
2	SEP	H	558	2	9,9,10	1.41	1 (11%)	9,12,14	2.18	2 (22%)

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	SEP	E	558	2	-	0/5/8/10	0/0/0/0
2	SEP	F	558	2	-	0/5/8/10	0/0/0/0
2	SEP	G	558	2	-	0/5/8/10	0/0/0/0
2	SEP	H	558	2	-	0/5/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	558	SEP	P-O1P	2.95	1.60	1.50
2	E	558	SEP	P-O1P	2.98	1.60	1.50
2	G	558	SEP	P-O1P	2.99	1.60	1.50
2	H	558	SEP	P-O1P	3.02	1.61	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	558	SEP	P-OG-CB	-4.07	107.08	118.30
2	E	558	SEP	P-OG-CB	-3.92	107.49	118.30
2	G	558	SEP	P-OG-CB	-3.89	107.59	118.30
2	F	558	SEP	P-OG-CB	-3.85	107.69	118.30
2	F	558	SEP	OG-CB-CA	3.90	112.01	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	558	SEP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	443:GLY	C	444:ARG	N	3.27

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	572/574 (99%)	-0.16	0 100 100	50, 92, 150, 189	0
1	B	567/574 (98%)	-0.07	7 (1%) 79 61	56, 114, 182, 213	0
1	C	554/574 (96%)	0.17	21 (3%) 41 20	73, 139, 215, 245	0
1	D	571/574 (99%)	0.02	9 (1%) 72 51	74, 124, 171, 207	0
2	E	17/18 (94%)	-0.21	0 100 100	114, 147, 167, 169	0
2	F	17/18 (94%)	0.18	1 (5%) 23 10	175, 195, 208, 210	0
2	G	17/18 (94%)	0.19	1 (5%) 23 10	182, 191, 240, 251	0
2	H	17/18 (94%)	0.21	1 (5%) 23 10	138, 167, 206, 208	0
All	All	2332/2368 (98%)	-0.01	40 (1%) 70 49	50, 119, 200, 251	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	456	LYS	4.5
1	D	18	LEU	4.4
2	G	563	PHE	4.4
1	C	454	GLU	4.2
1	D	50	VAL	4.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SEP	F	558	10/11	0.87	0.08	-	195,200,210,213	0
2	SEP	H	558	10/11	0.88	0.15	-	172,182,188,190	0
2	SEP	E	558	10/11	0.91	0.09	-	134,148,157,158	0
2	SEP	G	558	10/11	0.93	0.08	-	184,190,200,203	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.