



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:38 AM GMT

PDB ID : 2B05
Title : Crystal Structure of 14-3-3 gamma in complex with a phosphoserine peptide
Authors : Papagrigoriou, E.; Elkins, J.; Arrowsmith, C.; Zhao, Y.; Debreczeni, E.J.;
Edwards, A.; Weigelt, J.; Doyle, D.; von Delft, F.; Turnbull, A.; Yang, X.
Deposited on : 2005-09-13
Resolution : 2.55 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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

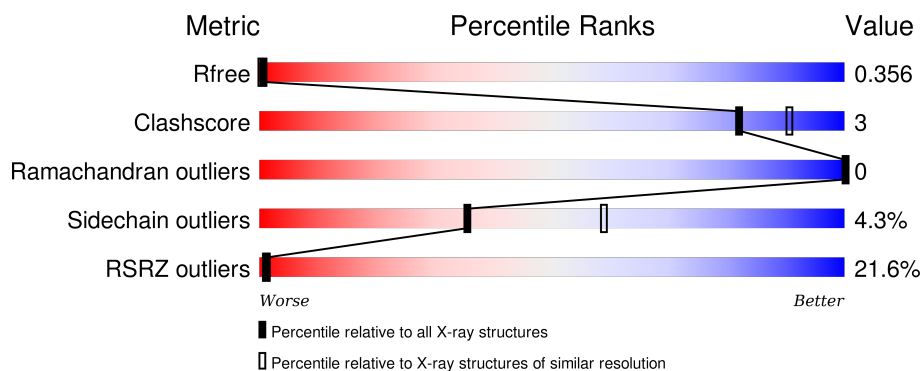
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	246	<div> <div>13%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
1	B	246	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
1	C	246	<div> <div>10%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
1	D	246	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>5%</div> </div> </div>
1	E	246	<div> <div>13%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	246	<div><div></div><div>72%</div><div></div><div>89%</div><div></div><div>6%</div><div>6%</div></div>
2	G	6	<div><div></div><div>50%</div><div></div><div>100%</div></div>
2	H	6	<div><div></div><div>17%</div><div></div><div>100%</div></div>
2	I	6	<div><div></div><div>83%</div><div></div><div>17%</div></div>
2	J	6	<div><div></div><div>17%</div><div></div><div>83%</div><div></div><div>17%</div></div>
2	K	6	<div><div></div><div>67%</div><div></div><div>17%</div><div></div><div>17%</div></div>
2	L	6	<div><div></div><div>83%</div><div></div><div>100%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11088 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 14-3-3 protein gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	2	0
			1823	1149	309	356	9			
1	B	233	Total	C	N	O	S	0	0	0
			1803	1134	303	357	9			
1	C	233	Total	C	N	O	S	0	0	0
			1802	1132	307	354	9			
1	D	233	Total	C	N	O	S	0	0	0
			1763	1107	303	344	9			
1	E	231	Total	C	N	O	S	0	0	0
			1729	1089	297	335	8			
1	F	232	Total	C	N	O	S	0	0	0
			1781	1122	300	350	9			

- Molecule 2 is a protein called peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	6	Total	C	N	O	P	0	0	0
			44	26	6	11	1			
2	H	6	Total	C	N	O	P	0	0	0
			44	26	6	11	1			
2	I	6	Total	C	N	O	P	0	0	0
			44	26	6	11	1			
2	J	6	Total	C	N	O	P	0	0	0
			44	26	6	11	1			
2	K	5	Total	C	N	O	P	0	0	0
			39	23	5	10	1			
2	L	6	Total	C	N	O	P	0	0	0
			44	26	6	11	1			

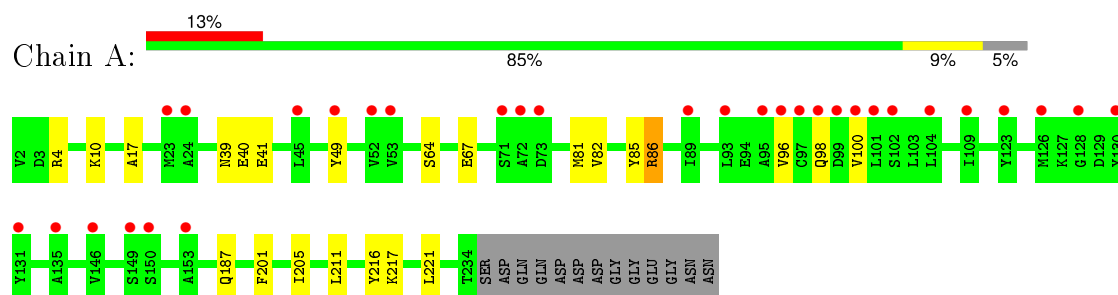
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total 35	O 35	0	3
3	B	20	Total 20	O 20	0	0
3	C	37	Total 37	O 37	0	0
3	D	19	Total 19	O 19	0	0
3	E	7	Total 7	O 7	0	0
3	G	2	Total 2	O 2	0	0
3	H	3	Total 3	O 3	0	0
3	I	2	Total 2	O 2	0	0
3	J	2	Total 2	O 2	0	0
3	K	1	Total 1	O 1	0	0

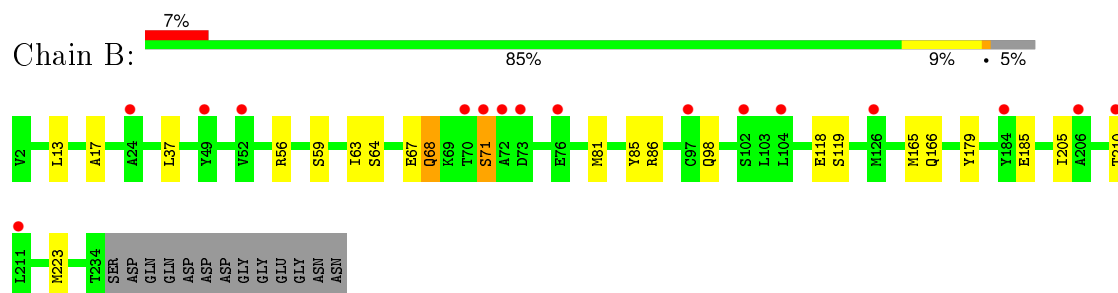
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

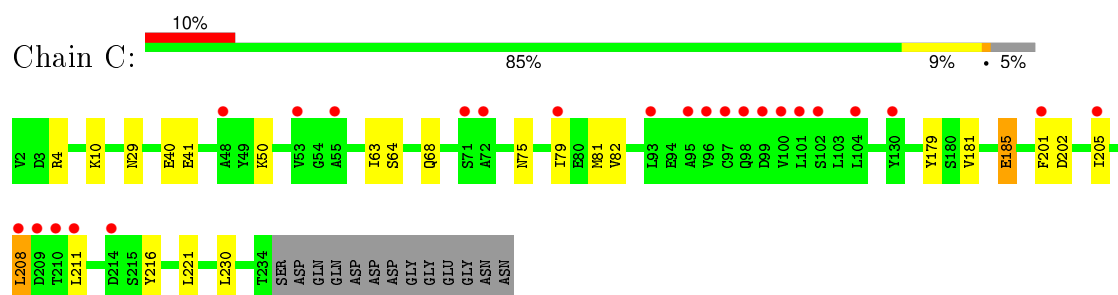
- Molecule 1: 14-3-3 protein gamma



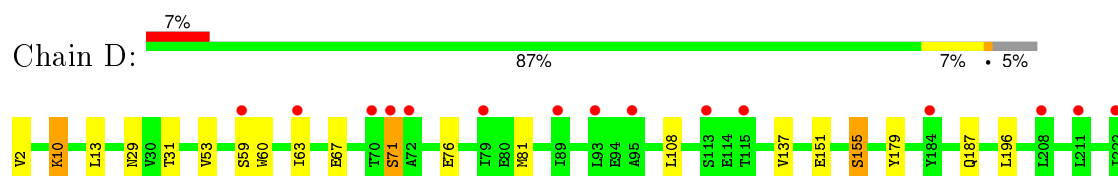
- Molecule 1: 14-3-3 protein gamma



- Molecule 1: 14-3-3 protein gamma

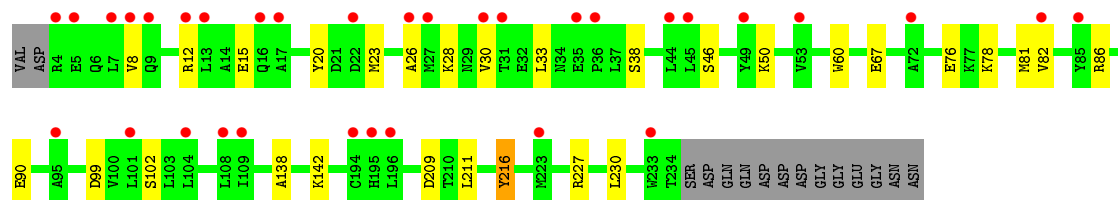
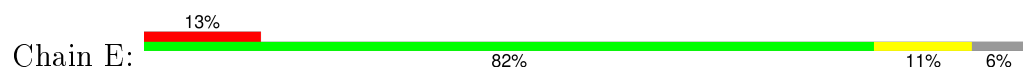


- Molecule 1: 14-3-3 protein gamma

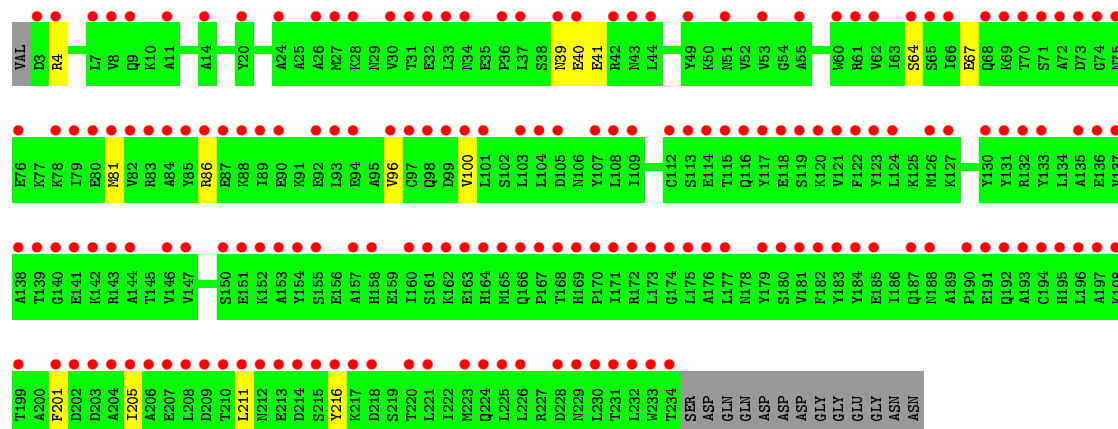
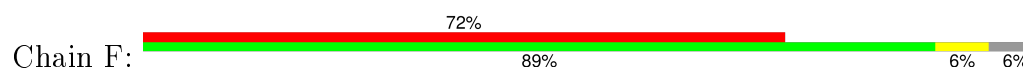




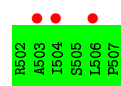
- Molecule 1: 14-3-3 protein gamma



- Molecule 1: 14-3-3 protein gamma



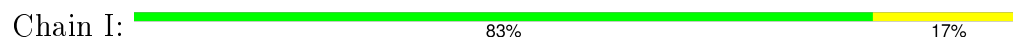
- Molecule 2: peptide



- Molecule 2: peptide

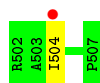
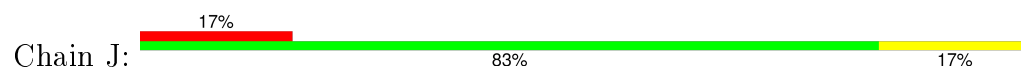


- Molecule 2: peptide

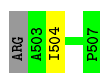




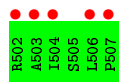
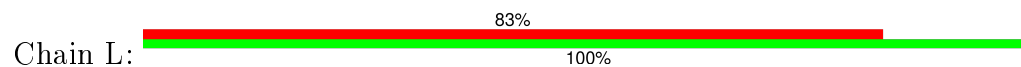
- Molecule 2: peptide



- Molecule 2: peptide



- Molecule 2: peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	121.57Å 121.57Å 313.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.20 – 2.55 48.22 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.20-2.55) 99.6 (48.22-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.258 , 0.302 0.329 , 0.356	Depositor DCC
R_{free} test set	2297 reflections (2.98%)	DCC
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 77107 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	11088	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.58	0/1859	0.62	1/2519 (0.0%)
1	B	0.63	0/1831	0.68	0/2484
1	C	0.60	0/1829	0.70	0/2479
1	D	0.54	0/1788	0.63	0/2428
1	E	0.53	0/1755	0.65	0/2387
1	F	0.37	0/1809	0.49	0/2455
2	G	0.47	0/33	0.40	0/42
2	H	0.63	0/33	0.60	0/42
2	I	1.64	1/33 (3.0%)	0.81	0/42
2	J	0.60	0/33	0.76	0/42
2	K	0.66	0/28	0.77	0/35
2	L	0.35	0/33	0.35	0/42
All	All	0.56	1/11064 (0.0%)	0.63	1/14997 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	507	PRO	C-OXT	8.56	1.39	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	86	ARG	NE-CZ-NH1	-5.51	117.54	120.30

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	1823	0	1745	14	0
1	B	1803	0	1700	13	0
1	C	1802	0	1711	15	0
1	D	1763	0	1657	11	0
1	E	1729	0	1608	15	0
1	F	1781	0	1673	6	0
2	G	44	0	38	0	0
2	H	44	0	38	0	0
2	I	44	0	38	0	0
2	J	44	0	38	0	0
2	K	39	0	36	0	0
2	L	44	0	39	0	0
3	A	35	0	0	1	0
3	B	20	0	0	0	0
3	C	37	0	0	1	0
3	D	19	0	0	0	0
3	E	7	0	0	0	0
3	G	2	0	0	0	0
3	H	3	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	1	0	0	0	0
All	All	11088	0	10321	67	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 3.

All (67) 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:B:98:GLN:HG3	1:D:2:VAL:HG21	1.32	1.08
1:C:201:PHE:CE2	1:C:205:ILE:HD11	2.07	0.90
1:C:75:ASN:O	1:C:79:ILE:HG13	1.74	0.88
1:A:17:ALA:HB2	1:D:63:ILE:HD11	1.56	0.88
1:B:166:GLN:HE22	1:B:210:THR:HB	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLN:NE2	1:B:210:THR:HB	1.91	0.83
1:A:201:PHE:CE2	1:A:205:ILE:HD12	2.20	0.75
1:E:15:GLU:HA	1:E:23:MET:HE2	1.70	0.74
1:E:20:TYR:CD1	1:E:23:MET:HE3	2.26	0.70
1:D:67:GLU:O	1:D:71:SER:HB2	1.94	0.68
1:A:85:TYR:CD1	1:D:10:LYS:HE2	2.29	0.68
1:E:20:TYR:HD1	1:E:23:MET:HE3	1.59	0.67
1:E:67:GLU:OE1	1:E:86:ARG:HD3	1.99	0.63
1:F:201:PHE:CE2	1:F:205:ILE:HD12	2.34	0.62
1:E:60:TRP:HE1	1:E:90:GLU:HG3	1.65	0.61
1:C:181:VAL:HG13	1:C:185:GLU:HG3	1.82	0.61
1:A:201:PHE:CE2	1:A:205:ILE:CD1	2.83	0.61
1:E:78:LYS:O	1:E:82:VAL:HG23	2.02	0.59
1:E:60:TRP:NE1	1:E:90:GLU:HG3	2.18	0.59
1:E:26:ALA:O	1:E:30:VAL:HG23	2.05	0.56
1:C:208:LEU:O	1:C:211:LEU:HG	2.05	0.56
1:C:201:PHE:CD2	1:C:205:ILE:HD11	2.40	0.55
1:D:187:GLN:HA	1:D:187:GLN:OE1	2.06	0.55
1:E:138:ALA:HB1	1:E:142:LYS:HG2	1.88	0.54
1:A:10:LYS:HD3	3:A:275:HOH:O	2.08	0.53
1:E:15:GLU:CA	1:E:23:MET:HE2	2.38	0.53
1:E:15:GLU:HA	1:E:23:MET:CE	2.37	0.53
1:B:64:SER:O	1:B:68:GLN:HG2	2.08	0.53
1:C:64:SER:O	1:C:68:GLN:HG2	2.08	0.53
1:D:31:THR:HG23	1:D:108:LEU:HD21	1.91	0.51
1:C:202:ASP:HA	1:C:205:ILE:HD12	1.91	0.51
1:F:67:GLU:OE1	1:F:86:ARG:HD3	2.11	0.50
1:C:4:ARG:HH21	1:C:41:GLU:CD	2.16	0.49
1:F:96:VAL:O	1:F:100:VAL:HG23	2.12	0.49
1:A:211:LEU:HD22	1:A:216:TYR:HA	1.95	0.49
1:B:67:GLU:OE1	1:B:86:ARG:HD3	2.13	0.49
1:A:49:TYR:CD1	1:A:100:VAL:HG22	2.48	0.48
1:F:211:LEU:HD22	1:F:216:TYR:HA	1.95	0.48
1:B:205:ILE:HG13	1:B:223:MET:HE1	1.96	0.48
1:D:60:TRP:CE2	1:D:137:VAL:HG12	2.49	0.47
1:E:211:LEU:HD22	1:E:216:TYR:HA	1.94	0.47
1:A:67:GLU:OE1	1:A:86:ARG:HD3	2.14	0.47
1:B:13:LEU:HD11	1:C:82:VAL:HG22	1.95	0.47
1:B:85:TYR:CD1	1:C:10:LYS:HE3	2.50	0.47
1:B:59:SER:O	1:B:63:ILE:HG12	2.14	0.47
1:B:67:GLU:O	1:B:71:SER:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:HH21	1:A:41:GLU:CD	2.19	0.46
1:A:82:VAL:HG22	1:D:13:LEU:HD11	1.98	0.46
1:F:201:PHE:CE2	1:F:205:ILE:CD1	2.99	0.45
1:D:59:SER:O	1:D:63:ILE:HG12	2.16	0.45
1:E:46:SER:O	1:E:50:LYS:HB2	2.17	0.45
1:A:187:GLN:OE1	1:A:187:GLN:HA	2.17	0.45
1:B:118:GLU:HA	1:B:165:MET:CE	2.46	0.44
1:C:201:PHE:CZ	1:C:205:ILE:HD11	2.52	0.43
1:C:10:LYS:NZ	3:C:262:HOH:O	2.51	0.43
1:C:205:ILE:HA	1:C:208:LEU:HD13	2.00	0.42
1:B:166:GLN:NE2	1:B:210:THR:CB	2.73	0.42
1:A:4:ARG:NH2	1:A:41:GLU:OE1	2.51	0.42
1:D:151:GLU:O	1:D:155:SER:HB2	2.19	0.42
1:E:30:VAL:HA	1:E:33:LEU:HD12	2.02	0.42
1:D:179:TYR:HB3	1:D:196:LEU:HD21	2.02	0.41
1:B:17:ALA:HB2	1:C:63:ILE:HD11	2.01	0.41
1:A:217:LYS:O	1:A:221[A]:LEU:HG	2.21	0.41
1:F:4:ARG:HH21	1:F:41:GLU:CD	2.23	0.41
1:C:4:ARG:NH2	1:C:41:GLU:OE1	2.48	0.41
1:A:96:VAL:O	1:A:100:VAL:HG23	2.21	0.41
1:E:8:VAL:HG12	1:E:12:ARG:CZ	2.51	0.40

There are no symmetry-related clashes.

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	233/246 (95%)	230 (99%)	3 (1%)	0	100	100
1	B	231/246 (94%)	227 (98%)	4 (2%)	0	100	100
1	C	231/246 (94%)	226 (98%)	5 (2%)	0	100	100
1	D	231/246 (94%)	227 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	229/246 (93%)	225 (98%)	4 (2%)	0	100	100
1	F	230/246 (94%)	227 (99%)	3 (1%)	0	100	100
2	G	3/6 (50%)	3 (100%)	0	0	100	100
2	H	3/6 (50%)	3 (100%)	0	0	100	100
2	I	3/6 (50%)	3 (100%)	0	0	100	100
2	J	3/6 (50%)	3 (100%)	0	0	100	100
2	K	2/6 (33%)	2 (100%)	0	0	100	100
2	L	3/6 (50%)	3 (100%)	0	0	100	100
All	All	1402/1512 (93%)	1379 (98%)	23 (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	185/215 (86%)	179 (97%)	6 (3%)	46	72
1	B	180/215 (84%)	172 (96%)	8 (4%)	35	58
1	C	180/215 (84%)	170 (94%)	10 (6%)	26	45
1	D	171/215 (80%)	164 (96%)	7 (4%)	37	61
1	E	164/215 (76%)	154 (94%)	10 (6%)	23	40
1	F	175/215 (81%)	171 (98%)	4 (2%)	58	82
2	G	3/4 (75%)	3 (100%)	0	100	100
2	H	3/4 (75%)	3 (100%)	0	100	100
2	I	3/4 (75%)	3 (100%)	0	100	100
2	J	3/4 (75%)	2 (67%)	1 (33%)	0	0
2	K	3/4 (75%)	2 (67%)	1 (33%)	0	0
2	L	3/4 (75%)	3 (100%)	0	100	100
All	All	1073/1314 (82%)	1026 (96%)	47 (4%)	35	58

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	40	GLU
1	A	64	SER
1	A	81	MET
1	A	98[A]	GLN
1	A	98[B]	GLN
1	B	37	LEU
1	B	56	ARG
1	B	68	GLN
1	B	71	SER
1	B	81	MET
1	B	119	SER
1	B	179	TYR
1	B	185	GLU
1	C	29	ASN
1	C	40	GLU
1	C	50	LYS
1	C	81	MET
1	C	179	TYR
1	C	185	GLU
1	C	208	LEU
1	C	216	TYR
1	C	221	LEU
1	C	230	LEU
1	D	10	LYS
1	D	29	ASN
1	D	53	VAL
1	D	71	SER
1	D	76	GLU
1	D	81	MET
1	D	155	SER
2	J	504	ILE
1	E	28	LYS
1	E	38	SER
1	E	76	GLU
1	E	81	MET
1	E	99	ASP
1	E	102	SER
1	E	209	ASP
1	E	216	TYR
1	E	227	ARG
1	E	230	LEU

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Mol	Chain	Res	Type
2	K	504	ILE
1	F	39	ASN
1	F	40	GLU
1	F	64	SER
1	F	81	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	B	68	GLN
1	B	166	GLN
1	C	68	GLN
1	D	68	GLN
1	F	29	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	G	505	2	8,9,10	1.45	1 (12%)	8,12,14	1.33	2 (25%)
2	SEP	H	505	2	8,9,10	1.45	1 (12%)	8,12,14	1.34	1 (12%)
2	SEP	I	505	2	8,9,10	1.45	1 (12%)	8,12,14	1.29	1 (12%)
2	SEP	J	505	2	8,9,10	1.46	1 (12%)	8,12,14	1.07	0
2	SEP	K	505	2	8,9,10	1.63	2 (25%)	8,12,14	1.42	1 (12%)
2	SEP	L	505	2	8,9,10	1.50	1 (12%)	8,12,14	1.48	2 (25%)

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	G	505	2	-	0/6/8/10	0/0/0/0
2	SEP	H	505	2	-	0/6/8/10	0/0/0/0
2	SEP	I	505	2	-	0/6/8/10	0/0/0/0
2	SEP	J	505	2	-	0/6/8/10	0/0/0/0
2	SEP	K	505	2	-	0/6/8/10	0/0/0/0
2	SEP	L	505	2	-	0/6/8/10	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	505	SEP	P-O2P	2.35	1.63	1.54
2	J	505	SEP	P-O1P	2.72	1.60	1.51
2	I	505	SEP	P-O1P	2.79	1.60	1.51
2	L	505	SEP	P-O1P	2.95	1.60	1.51
2	H	505	SEP	P-O1P	3.03	1.61	1.51
2	K	505	SEP	P-O1P	3.35	1.62	1.51
2	G	505	SEP	P-O1P	3.38	1.62	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	505	SEP	O-C-CA	-2.36	119.34	125.49
2	I	505	SEP	O-C-CA	-2.23	119.68	125.49
2	G	505	SEP	O-C-CA	-2.19	119.80	125.49
2	H	505	SEP	O-C-CA	-2.15	119.88	125.49
2	L	505	SEP	O-C-CA	-2.08	120.08	125.49
2	G	505	SEP	OG-CB-CA	2.33	110.26	108.27
2	L	505	SEP	OG-CB-CA	2.77	110.64	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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, 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	233/246 (94%)	1.04	31 (13%) 4 5	30, 56, 67, 78	0
1	B	233/246 (94%)	0.92	16 (6%) 20 23	30, 56, 70, 75	0
1	C	233/246 (94%)	0.88	24 (10%) 9 9	30, 56, 72, 76	0
1	D	233/246 (94%)	0.68	16 (6%) 20 23	25, 56, 69, 75	0
1	E	231/246 (93%)	0.87	33 (14%) 4 4	24, 57, 64, 70	0
1	F	232/246 (94%)	4.03	178 (76%) 0 0	30, 58, 67, 72	0
2	G	5/6 (83%)	1.64	3 (60%) 0 0	59, 62, 70, 72	0
2	H	5/6 (83%)	2.08	1 (20%) 1 1	56, 64, 69, 71	0
2	I	5/6 (83%)	0.71	0 100 100	26, 61, 68, 70	0
2	J	5/6 (83%)	1.12	1 (20%) 1 1	57, 60, 65, 68	0
2	K	4/6 (66%)	1.17	0 100 100	56, 59, 61, 64	0
2	L	5/6 (83%)	5.91	5 (100%) 0 0	66, 67, 68, 68	0
All	All	1424/1512 (94%)	1.42	308 (21%) 1 1	24, 57, 69, 78	0

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	181	VAL	13.8
1	F	79	ILE	13.2
1	F	211	LEU	13.0
1	F	210	THR	12.1
1	F	135	ALA	11.7
1	F	179	TYR	10.8
1	F	85	TYR	10.2
1	F	208	LEU	9.9
1	F	140	GLY	9.3
1	F	204	ALA	9.2
1	F	78	LYS	9.0

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Mol	Chain	Res	Type	RSRZ
1	F	232	LEU	8.9
1	B	71	SER	8.5
1	F	201	PHE	8.4
1	F	96	VAL	8.3
1	B	70	THR	8.2
2	L	504	ILE	8.1
1	F	76	GLU	8.0
1	F	103	LEU	8.0
1	F	124	LEU	7.9
1	F	109	ILE	7.8
1	F	163	GLU	7.8
1	F	183	TYR	7.7
1	F	139	THR	7.6
1	F	209	ASP	7.5
1	F	115	THR	7.4
1	F	117	TYR	7.4
2	L	506	LEU	7.4
1	F	197	ALA	7.4
1	F	230	LEU	7.2
1	F	223	MET	7.2
1	F	167	PRO	7.2
1	F	138	ALA	7.1
1	F	164	HIS	7.0
1	F	27	MET	7.0
1	F	168	THR	6.7
2	L	502	ARG	6.5
1	F	86	ARG	6.5
1	F	72	ALA	6.5
1	F	176	ALA	6.5
1	F	206	ALA	6.4
1	F	165	MET	6.4
1	F	71	SER	6.4
1	F	30	VAL	6.4
1	F	120	LYS	6.2
1	F	118	GLU	6.2
1	F	97	CYS	6.1
1	F	121	VAL	6.1
1	F	101	LEU	6.0
1	F	194	CYS	5.9
1	F	105	ASP	5.9
1	F	123	TYR	5.9
1	F	172	ARG	5.8

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Mol	Chain	Res	Type	RSRZ
1	F	214	ASP	5.8
1	C	71	SER	5.8
1	F	94	GLU	5.7
1	F	217	LYS	5.6
1	F	82	VAL	5.6
1	F	195	HIS	5.6
1	F	26	ALA	5.5
1	F	221	LEU	5.5
1	F	100	VAL	5.5
1	F	31	THR	5.5
1	F	175	LEU	5.4
1	F	122	PHE	5.4
1	F	233	TRP	5.4
1	F	141	GLU	5.4
1	F	80	GLU	5.4
1	F	64	SER	5.3
1	F	231	THR	5.3
1	F	171	ILE	5.3
1	F	137	VAL	5.2
1	F	202	ASP	5.2
1	F	104	LEU	5.1
1	F	81	MET	5.1
1	F	212	ASN	5.1
1	F	166	GLN	5.1
1	F	144	ALA	5.1
1	F	215	SER	5.1
1	F	98	GLN	5.1
1	F	177	LEU	5.0
1	F	24	ALA	5.0
1	F	113	SER	5.0
1	F	60	TRP	4.8
1	F	73	ASP	4.8
1	F	226	LEU	4.8
2	H	502	ARG	4.8
1	F	154	TYR	4.8
1	E	8	VAL	4.7
1	F	207	GLU	4.7
1	B	72	ALA	4.7
1	F	131	TYR	4.6
1	C	205	ILE	4.6
1	E	17	ALA	4.6
1	F	173	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	174	GLY	4.5
1	F	33	LEU	4.5
1	F	108	LEU	4.5
1	C	214	ASP	4.4
1	F	187	GLN	4.4
1	D	71	SER	4.4
1	F	136	GLU	4.4
1	F	143	ARG	4.3
1	F	133	TYR	4.3
1	F	160	ILE	4.3
1	F	170	PRO	4.3
1	F	68	GLN	4.3
1	A	72	ALA	4.2
1	F	234	THR	4.2
1	F	112	CYS	4.2
1	F	61	ARG	4.2
1	F	83	ARG	4.2
1	F	62	VAL	4.2
1	F	126	MET	4.1
1	F	155	SER	4.1
1	F	44	LEU	4.1
1	F	169	HIS	4.1
1	F	191	GLU	4.0
1	F	213	GLU	4.0
1	F	70	THR	4.0
1	F	157	ALA	4.0
1	F	37	LEU	4.0
1	A	97	CYS	4.0
1	F	119	SER	4.0
1	F	65	SER	3.9
1	F	188	ASN	3.9
1	E	26	ALA	3.9
1	C	210	THR	3.8
1	F	184	TYR	3.8
1	F	127	LYS	3.8
2	L	503	ALA	3.8
1	F	36	PRO	3.8
1	A	95	ALA	3.7
1	F	205	ILE	3.7
2	L	507	PRO	3.7
1	F	66	ILE	3.6
1	C	95	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	75	ASN	3.6
1	F	218	ASP	3.6
1	E	5	GLU	3.6
1	B	206	ALA	3.6
1	F	142	LYS	3.6
1	F	28	LYS	3.6
1	F	99	ASP	3.5
1	F	216	TYR	3.5
1	F	180	SER	3.5
1	F	225	LEU	3.4
1	F	153	ALA	3.4
1	A	73	ASP	3.4
1	F	34	ASN	3.4
1	A	131	TYR	3.4
1	F	53	VAL	3.3
1	F	130	TYR	3.3
1	F	185	GLU	3.3
1	F	190	PRO	3.3
1	F	74	GLY	3.3
1	A	101	LEU	3.2
1	E	36	PRO	3.2
1	F	7	LEU	3.2
1	F	40	GLU	3.2
1	F	151	GLU	3.2
1	C	72	ALA	3.2
1	F	228	ASP	3.2
1	E	7	LEU	3.2
1	C	97	CYS	3.1
1	D	70	THR	3.1
1	F	49	TYR	3.1
1	F	3	ASP	3.1
1	C	100	VAL	3.1
1	F	158	HIS	3.1
1	A	96	VAL	3.1
1	A	100	VAL	3.1
1	F	146	VAL	3.1
1	E	12	ARG	3.1
1	F	203	ASP	3.1
1	F	69	LYS	3.1
1	E	16	GLN	3.0
1	F	4	ARG	3.0
1	F	147	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	11	ALA	3.0
1	C	208	LEU	3.0
1	E	72	ALA	3.0
1	F	32	GLU	3.0
1	F	89	ILE	2.9
1	A	98[A]	GLN	2.9
1	F	8	VAL	2.9
1	F	152	LYS	2.9
1	D	233	TRP	2.9
1	E	85	TYR	2.8
1	F	93	LEU	2.8
1	F	116	GLN	2.8
1	F	229	ASN	2.8
1	B	210	THR	2.8
1	F	220	THR	2.8
1	B	76	GLU	2.8
1	B	73	ASP	2.8
1	E	22	ASP	2.8
1	E	82	VAL	2.8
1	C	211	LEU	2.8
1	E	196	LEU	2.8
1	B	52	VAL	2.8
1	E	30	VAL	2.8
1	F	224	GLN	2.7
1	E	49	TYR	2.7
1	C	130	TYR	2.6
1	D	184	TYR	2.6
1	C	79	ILE	2.6
1	E	13	LEU	2.6
1	E	4	ARG	2.6
1	C	209	ASP	2.6
1	E	233	TRP	2.6
1	A	128	GLY	2.5
1	F	196	LEU	2.5
1	D	72	ALA	2.5
1	F	193	ALA	2.5
1	F	87	GLU	2.5
1	F	192	GLN	2.5
1	F	198	LYS	2.5
1	B	97	CYS	2.5
1	E	95	ALA	2.5
1	E	45	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	114	GLU	2.5
1	D	63	ILE	2.5
1	F	43	ASN	2.5
1	E	9	GLN	2.5
1	F	92	GLU	2.4
1	F	150	SER	2.4
1	C	104	LEU	2.4
1	A	93	LEU	2.4
1	D	93	LEU	2.4
1	A	71	SER	2.4
1	A	99	ASP	2.4
1	E	195	HIS	2.4
1	C	93	LEU	2.4
1	E	44	LEU	2.4
1	D	59	SER	2.4
1	F	182	PHE	2.4
1	D	208	LEU	2.4
1	E	223	MET	2.4
1	F	39	ASN	2.3
1	A	130	TYR	2.3
1	E	35	GLU	2.3
1	E	53	VAL	2.3
2	J	504	ILE	2.3
1	E	108	LEU	2.3
1	F	88	LYS	2.3
1	A	45	LEU	2.3
1	A	102	SER	2.3
1	B	184	TYR	2.3
1	C	102	SER	2.3
1	A	153	ALA	2.3
1	B	102	SER	2.3
1	A	123	TYR	2.3
2	G	504	ILE	2.3
1	C	53	VAL	2.3
1	A	89	ILE	2.2
1	A	135	ALA	2.2
1	C	48	ALA	2.2
1	F	51	ASN	2.2
1	A	104	LEU	2.2
1	C	99	ASP	2.2
1	C	101	LEU	2.2
1	F	20	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	55	ALA	2.2
1	A	150	SER	2.2
1	E	101	LEU	2.2
1	C	55	ALA	2.2
1	C	98	GLN	2.2
1	D	89	ILE	2.2
1	F	199	THR	2.2
1	A	53	VAL	2.2
1	C	96	VAL	2.2
1	B	24	ALA	2.2
1	F	84	ALA	2.2
1	A	126	MET	2.2
1	A	49	TYR	2.1
1	D	95	ALA	2.1
1	D	79	ILE	2.1
1	E	194	CYS	2.1
2	G	506	LEU	2.1
2	G	503	ALA	2.1
1	A	52	VAL	2.1
1	E	109	ILE	2.1
1	B	104	LEU	2.1
1	D	211	LEU	2.1
1	D	115	THR	2.1
1	A	24	ALA	2.1
1	A	23	MET	2.1
1	F	107	TYR	2.1
1	E	27	MET	2.1
1	A	109	ILE	2.1
1	D	222	ILE	2.1
1	E	31	THR	2.1
1	D	113	SER	2.1
1	F	14	ALA	2.1
1	B	211	LEU	2.1
1	F	161	SER	2.1
1	C	201	PHE	2.0
1	F	9	GLN	2.0
1	F	132	ARG	2.0
1	F	162	LYS	2.0
1	A	146	VAL	2.0
1	B	126	MET	2.0
1	B	49	TYR	2.0
1	F	90	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	149	SER	2.0
1	E	104	LEU	2.0
1	F	42	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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(Å ²)	Q<0.9
2	SEP	I	505	10/11	0.96	0.22	-	51,55,60,61	0
2	SEP	H	505	10/11	0.97	0.18	-	56,59,59,61	0
2	SEP	K	505	10/11	0.96	0.21	-	48,54,57,58	0
2	SEP	J	505	10/11	0.95	0.20	-	54,56,58,60	0
2	SEP	G	505	10/11	0.97	0.24	-	53,58,60,62	0
2	SEP	L	505	10/11	0.71	0.26	-	58,62,65,66	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.