



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:34 AM UTC

PDB ID : 2B05 / pdb_00002b05
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

<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

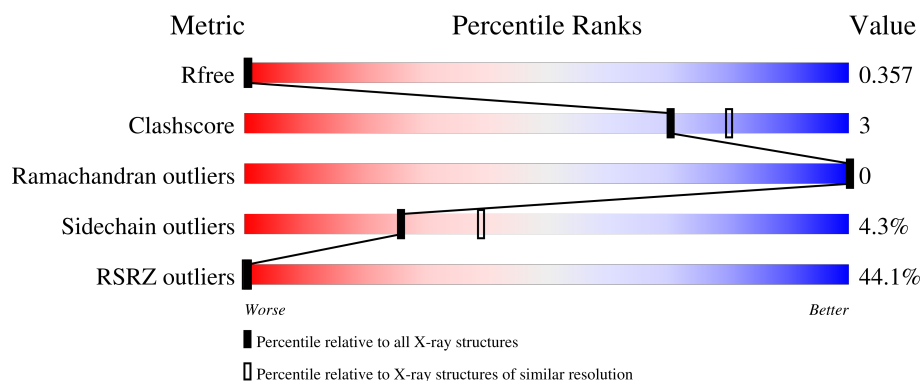
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	246	33% 85% 9% 5%
1	B	246	31% 85% 9% 5%
1	C	246	29% 83% 11% 5%
1	D	246	29% 86% 7% 5%
1	E	246	35% 81% 13% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	246	90% 88% 6% 6%
2	G	6	67% 83% 17%
2	H	6	67% 83% 17%
2	I	6	67% 67% 33%
2	J	6	33% 67% 33%
2	K	6	33% 50% 33% 17%
2	L	6	83% 83% 17%

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			

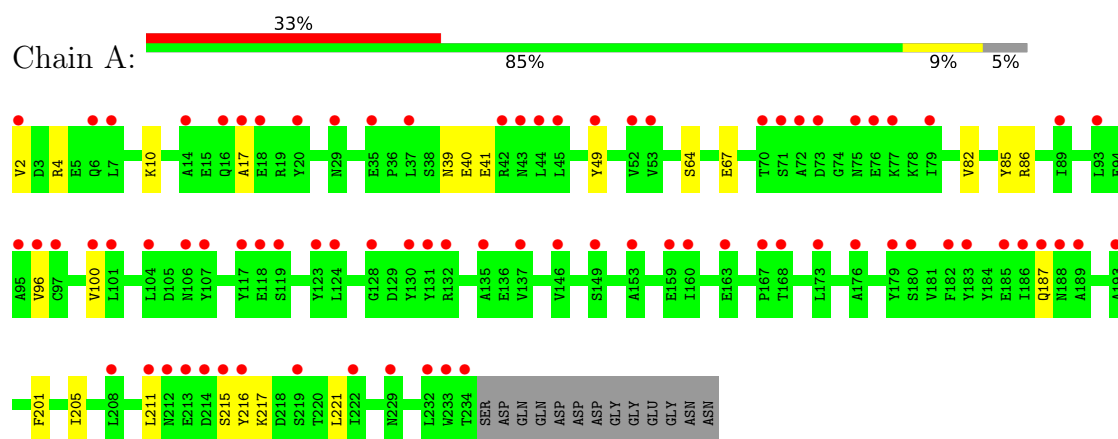
- Molecule 3 is water.

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

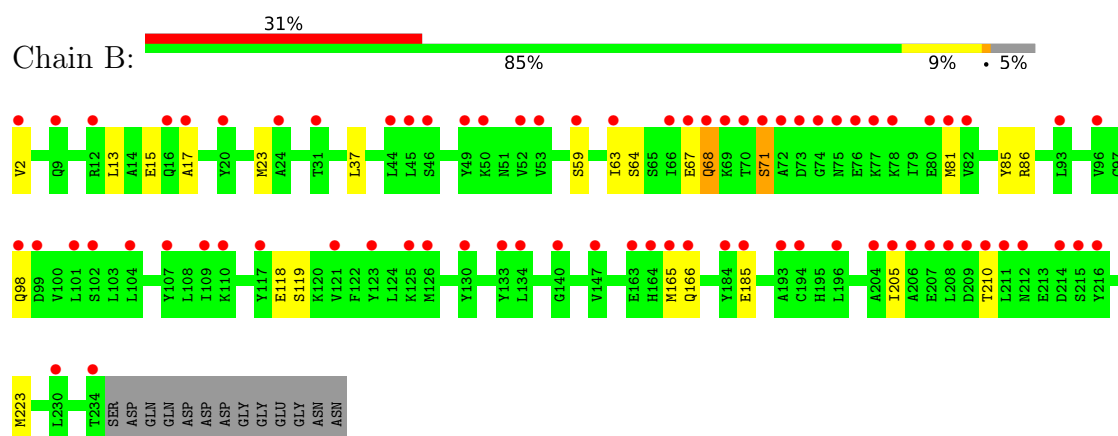
3 Residue-property plots [i](#)

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.

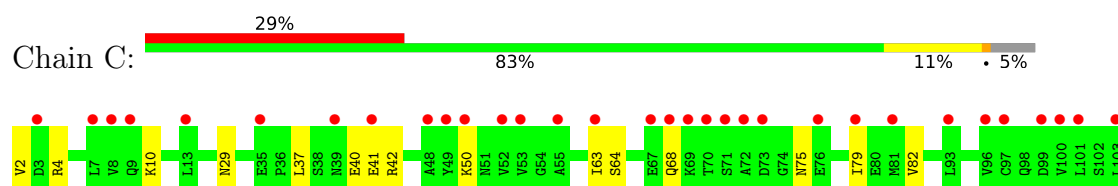
• Molecule 1: 14-3-3 protein gamma

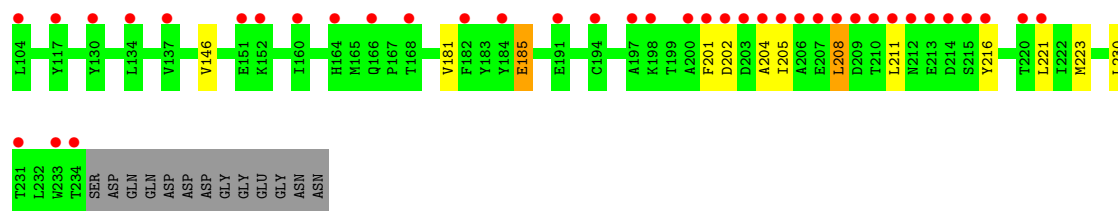


• Molecule 1: 14-3-3 protein gamma



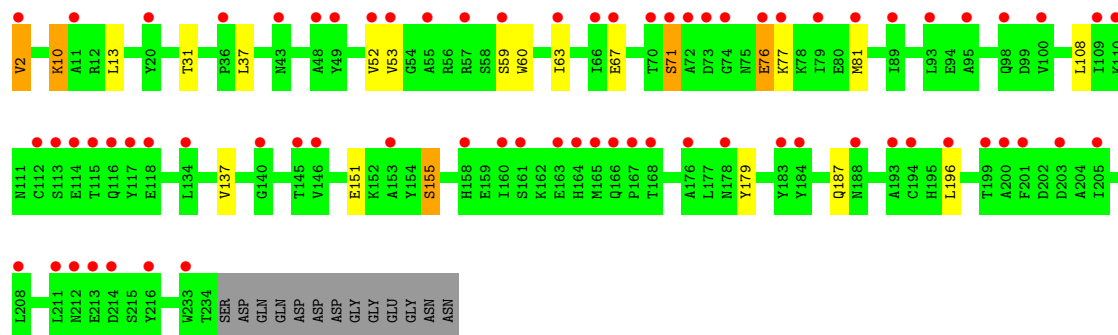
• Molecule 1: 14-3-3 protein gamma





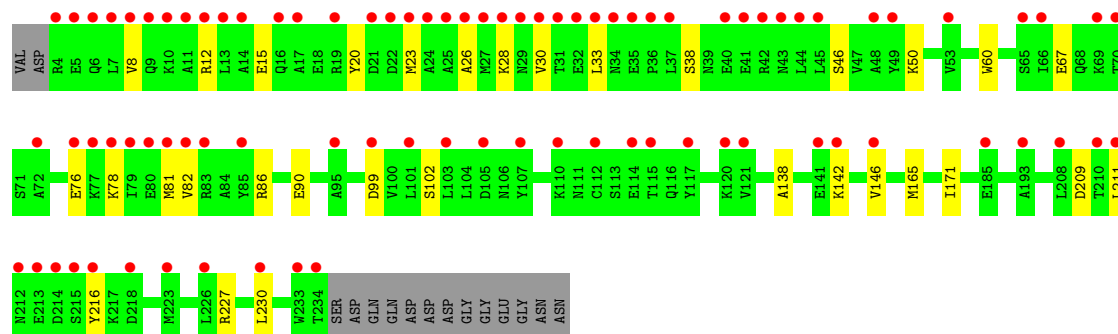
• Molecule 1: 14-3-3 protein gamma

Chain D: 29% 86% 7% 5%



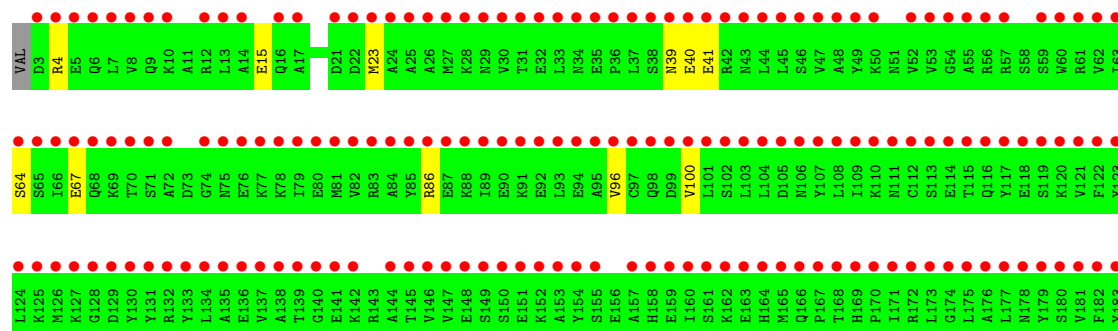
• Molecule 1: 14-3-3 protein gamma

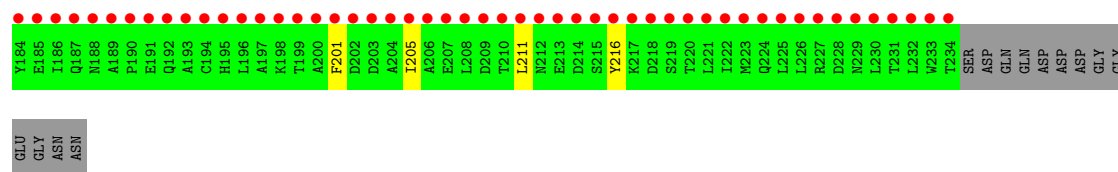
Chain E: 35% 81% 13% 6%



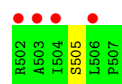
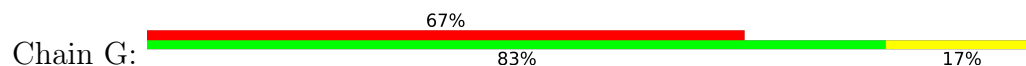
• Molecule 1: 14-3-3 protein gamma

Chain F: 90% 88% 6% 6%

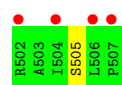
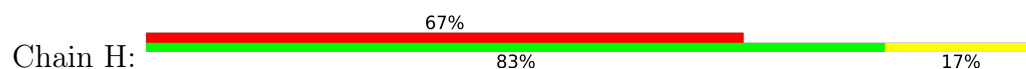




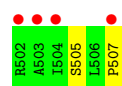
- Molecule 2: peptide



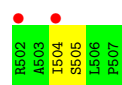
- Molecule 2: peptide



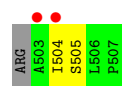
- Molecule 2: peptide



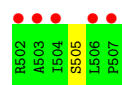
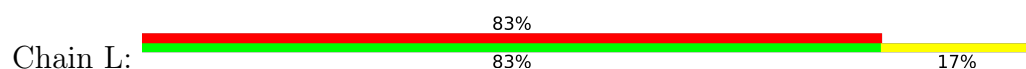
- Molecule 2: peptide



- 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 48.20 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.20-2.55) 99.6 (48.20-2.55)	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 0.334 , 0.357	Depositor DCC
R_{free} test set	2301 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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: 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	0.70	0/1859	0.88	0/2519
1	B	0.74	0/1831	0.94	0/2484
1	C	0.71	0/1829	0.93	0/2479
1	D	0.65	1/1788 (0.1%)	0.89	0/2428
1	E	0.67	0/1755	0.96	0/2387
1	F	0.48	0/1809	0.89	0/2455
2	G	0.56	0/33	0.51	0/42
2	H	0.70	0/33	0.65	0/42
2	I	1.57	1/33 (3.0%)	0.81	0/42
2	J	0.72	0/33	0.88	0/42
2	K	0.69	0/28	0.68	0/35
2	L	0.36	0/33	0.43	0/42
All	All	0.67	2/11064 (0.0%)	0.91	0/14997

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	507	PRO	C-OXT	8.04	1.39	1.23
1	D	52	VAL	CA-CB	5.15	1.60	1.54

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	1823	0	1745	15	0
1	B	1803	0	1700	14	0
1	C	1802	0	1711	16	0
1	D	1763	0	1657	12	0
1	E	1729	0	1608	16	0
1	F	1781	0	1673	7	0
2	G	44	0	39	0	0
2	H	44	0	39	0	0
2	I	44	0	39	0	0
2	J	44	0	39	0	0
2	K	39	0	37	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	10326	73	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 (73) 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:E:15:GLU:HA	1:E:23:MET:HE2	1.52	0.91
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
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:CA	1:E:23:MET:HE2	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:181:VAL:HG13	1:C:185:GLU:HG3	1.82	0.61
1:E:60:TRP:HE1	1:E:90:GLU:HG3	1.65	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:C:4:ARG:HH21	1:C:41:GLU:CD	2.16	0.54
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: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:A:4:ARG:HH21	1:A:41:GLU:CD	2.19	0.50
1:F:67:GLU:OE1	1:F:86:ARG:HD3	2.11	0.50
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:B:15:GLU:HB2	1:B:23:MET:HE3	1.95	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: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:C:204:ALA:HB3	1:C:223:MET:HE3	1.97	0.47
1:B:59:SER:O	1:B:63:ILE:HG12	2.14	0.47
1:E:20:TYR:CD1	1:E:23:MET:HE3	2.50	0.46
1:B:67:GLU:O	1:B:71:SER:HB3	2.15	0.46
1:A:82:VAL:HG22	1:D:13:LEU:HD11	1.98	0.46
1:F:4:ARG:HH21	1:F:41:GLU:CD	2.23	0.45
1:F:201:PHE:CE2	1:F:205:ILE:CD1	2.99	0.45
1:A:187:GLN:OE1	1:A:187:GLN:HA	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:118:GLU:HA	1:B:165:MET:CE	2.46	0.44
1:B:205:ILE:HG13	1:B:223:MET:HE1	2.00	0.44
1:C:201:PHE:CZ	1:C:205:ILE:HD11	2.52	0.43
1:D:76:GLU:O	1:D:77:LYS:C	2.60	0.43
1:E:15:GLU:HA	1:E:23:MET:CE	2.37	0.43
1:C:10:LYS:NZ	3:C:262:HOH:O	2.51	0.43
1:E:20:TYR:CD1	1:E:23:MET:CE	3.02	0.43
1:E:165:MET:HE1	1:E:171:ILE:HB	2.01	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:F:15:GLU:HB2	1:F:23:MET:HE3	2.02	0.41
1:A:215:SER:O	1:A:216:TYR:C	2.62	0.41
1:B:17:ALA:HB2	1:C:63:ILE:HD11	2.01	0.41
1:D:179:TYR:HB3	1:D:196:LEU:HD21	2.02	0.41
1:A:217:LYS:O	1:A:221[A]:LEU:HG	2.21	0.41
1:A:96:VAL:O	1:A:100:VAL:HG23	2.21	0.41
1:C:4:ARG:NH2	1:C:41:GLU:OE1	2.48	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	231/246 (94%)	226 (98%)	5 (2%)	0	100	100
1	D	231/246 (94%)	227 (98%)	4 (2%)	0	100	100
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%)	181 (98%)	4 (2%)	45	64
1	B	180/215 (84%)	173 (96%)	7 (4%)	28	43
1	C	180/215 (84%)	168 (93%)	12 (7%)	15	21
1	D	171/215 (80%)	163 (95%)	8 (5%)	23	36
1	E	164/215 (76%)	154 (94%)	10 (6%)	17	25
1	F	175/215 (81%)	172 (98%)	3 (2%)	53	72
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	3/4 (75%)	3 (100%)	0	100	100
All	All	1073/1314 (82%)	1027 (96%)	46 (4%)	26	39

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	39	ASN
1	A	40	GLU
1	A	64	SER
1	B	2	VAL
1	B	37	LEU
1	B	68	GLN
1	B	71	SER
1	B	81	MET
1	B	119	SER
1	B	185	GLU
1	C	2	VAL
1	C	29	ASN
1	C	37	LEU
1	C	40	GLU
1	C	42	ARG
1	C	50	LYS
1	C	146	VAL
1	C	185	GLU
1	C	208	LEU
1	C	216	TYR
1	C	221	LEU
1	C	230	LEU
1	D	2	VAL
1	D	10	LYS
1	D	37	LEU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	99	ASP
1	E	102	SER
1	E	146	VAL
1	E	209	ASP
1	E	227	ARG
1	E	230	LEU
2	K	504	ILE
1	F	39	ASN
1	F	40	GLU
1	F	64	SER

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

Mol	Chain	Res	Type
1	A	6	GLN
1	A	29	ASN
1	B	16	GLN
1	B	39	ASN
1	B	68	GLN
1	B	166	GLN
1	C	68	GLN
1	D	29	ASN
1	D	68	GLN
1	E	68	GLN
1	E	106	ASN
1	F	16	GLN
1	F	29	ASN
1	F	158	HIS

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	H	505	2	8,9,10	1.54	1 (12%)	7,12,14	1.25	1 (14%)
2	SEP	I	505	2	8,9,10	1.54	1 (12%)	7,12,14	1.09	0
2	SEP	G	505	2	8,9,10	1.58	1 (12%)	7,12,14	1.12	1 (14%)
2	SEP	K	505	2	8,9,10	1.74	2 (25%)	7,12,14	1.22	0
2	SEP	J	505	2	8,9,10	1.54	1 (12%)	7,12,14	0.87	0
2	SEP	L	505	2	8,9,10	1.59	1 (12%)	7,12,14	1.34	1 (14%)

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	H	505	2	-	0/6/8/10	-
2	SEP	I	505	2	-	1/6/8/10	-
2	SEP	G	505	2	-	0/6/8/10	-
2	SEP	K	505	2	-	0/6/8/10	-
2	SEP	J	505	2	-	0/6/8/10	-
2	SEP	L	505	2	-	0/6/8/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	505	SEP	P-O1P	3.80	1.62	1.50
2	K	505	SEP	P-O1P	3.76	1.62	1.50
2	H	505	SEP	P-O1P	3.43	1.61	1.50
2	L	505	SEP	P-O1P	3.34	1.60	1.50
2	I	505	SEP	P-O1P	3.18	1.60	1.50
2	J	505	SEP	P-O1P	3.10	1.60	1.50
2	K	505	SEP	P-O2P	2.25	1.63	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	505	SEP	OG-CB-CA	2.56	110.64	108.14
2	G	505	SEP	OG-CB-CA	2.18	110.26	108.14
2	H	505	SEP	O2P-P-OG	2.07	112.08	106.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	505	SEP	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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%)	1.80	80 (34%) 1 0	30, 56, 67, 78	2 (0%)
1	B	233/246 (94%)	1.85	76 (32%) 1 0	30, 56, 70, 75	0
1	C	233/246 (94%)	1.77	71 (30%) 1 0	30, 56, 72, 76	0
1	D	233/246 (94%)	1.65	72 (30%) 1 0	25, 56, 69, 75	0
1	E	231/246 (93%)	1.91	86 (37%) 1 0	24, 57, 64, 70	0
1	F	232/246 (94%)	3.92	222 (95%) 0 0	30, 58, 67, 72	0
2	G	5/6 (83%)	3.39	4 (80%) 0 0	59, 62, 70, 72	0
2	H	5/6 (83%)	2.98	4 (80%) 0 0	56, 64, 69, 71	0
2	I	5/6 (83%)	2.59	4 (80%) 0 0	26, 61, 68, 70	0
2	J	5/6 (83%)	2.02	2 (40%) 1 0	57, 60, 65, 68	0
2	K	4/6 (66%)	1.90	2 (50%) 0 0	56, 59, 61, 64	0
2	L	5/6 (83%)	4.49	5 (100%) 0 0	66, 67, 68, 68	0
All	All	1424/1512 (94%)	2.17	628 (44%) 0 0	24, 57, 69, 78	2 (0%)

All (628) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	THR	10.0
1	B	71	SER	9.4
1	F	79	ILE	8.4
1	F	76	GLU	8.2
1	F	179	TYR	7.0
1	D	71	SER	6.8
1	F	211	LEU	6.6
1	F	63	ILE	6.6
1	F	138	ALA	6.4
1	F	204	ALA	6.4
1	C	214	ASP	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	72	ALA	6.3
1	C	71	SER	6.3
1	F	201	PHE	6.2
1	B	76	GLU	6.2
1	F	104	LEU	6.1
1	F	134	LEU	6.1
1	F	230	LEU	6.1
1	F	124	LEU	6.0
1	F	181	VAL	6.0
1	F	223	MET	5.9
1	E	26	ALA	5.9
1	F	177	LEU	5.8
1	F	216	TYR	5.8
2	L	506	LEU	5.8
1	C	205	ILE	5.7
1	F	208	LEU	5.7
1	F	74	GLY	5.7
1	F	101	LEU	5.7
1	F	82	VAL	5.7
1	F	205	ILE	5.6
1	F	220	THR	5.6
2	L	504	ILE	5.6
1	B	80	GLU	5.5
1	F	135	ALA	5.5
1	F	78	LYS	5.5
1	F	175	LEU	5.5
1	F	123	TYR	5.4
1	A	73	ASP	5.4
1	F	85	TYR	5.4
1	F	214	ASP	5.4
1	E	27	MET	5.4
1	F	167	PRO	5.3
1	F	108	LEU	5.3
2	H	502	ARG	5.3
1	F	226	LEU	5.3
1	F	98	GLN	5.3
1	F	109	ILE	5.3
1	F	163	GLU	5.2
1	F	171	ILE	5.2
1	F	154	TYR	5.2
1	F	103	LEU	5.2
1	F	121	VAL	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	117	TYR	5.2
1	F	183	TYR	5.2
1	F	45	LEU	5.2
1	F	222	ILE	5.2
1	E	8	VAL	5.1
1	C	206	ALA	5.1
1	F	130	TYR	5.1
1	F	93	LEU	5.1
1	F	100	VAL	5.1
1	F	81	MET	5.0
1	C	210	THR	5.0
1	E	22	ASP	5.0
1	F	176	ALA	5.0
1	F	77	LYS	5.0
1	F	212	ASN	4.9
1	F	97	CYS	4.9
1	F	172	ARG	4.9
1	F	233	TRP	4.9
1	F	210	THR	4.9
1	B	206	ALA	4.9
1	F	213	GLU	4.9
1	F	30	VAL	4.9
1	F	225	LEU	4.9
1	F	122	PHE	4.8
1	E	17	ALA	4.8
1	F	199	THR	4.8
1	F	6	GLN	4.8
1	F	84	ALA	4.7
1	F	196	LEU	4.7
2	G	504	ILE	4.7
1	F	115	THR	4.7
1	F	192	GLN	4.7
1	F	195	HIS	4.7
1	F	142	LYS	4.7
1	C	208	LEU	4.6
1	E	107	TYR	4.6
1	F	197	ALA	4.6
1	C	209	ASP	4.6
1	F	186	ILE	4.5
1	F	70	THR	4.5
2	G	503	ALA	4.5
1	F	221	LEU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	232	LEU	4.5
1	D	72	ALA	4.5
1	F	137	VAL	4.5
1	F	96	VAL	4.4
1	F	165	MET	4.4
1	F	173	LEU	4.4
1	E	95	ALA	4.4
1	D	70	THR	4.4
1	F	145	THR	4.4
1	F	164	HIS	4.4
1	D	213	GLU	4.4
1	F	69	LYS	4.4
1	F	110	LYS	4.4
1	F	31	THR	4.3
1	F	159	GLU	4.3
1	D	214	ASP	4.3
1	F	75	ASN	4.3
1	F	174	GLY	4.3
1	C	72	ALA	4.3
1	F	126	MET	4.3
1	F	140	GLY	4.3
1	F	194	CYS	4.3
2	L	502	ARG	4.3
1	B	73	ASP	4.2
1	F	170	PRO	4.2
1	F	89	ILE	4.2
1	F	94	GLU	4.2
1	F	25	ALA	4.2
1	F	184	TYR	4.2
1	A	214	ASP	4.2
1	F	53	VAL	4.2
1	F	86	ARG	4.2
1	F	160	ILE	4.1
1	F	234	THR	4.1
1	B	69	LYS	4.1
1	F	120	LYS	4.1
1	A	72	ALA	4.1
1	E	29	ASN	4.1
1	F	105	ASP	4.1
1	E	13	LEU	4.1
1	F	127	LYS	4.1
1	C	211	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	72	ALA	4.1
1	F	200	ALA	4.1
1	F	217	LYS	4.1
1	F	27	MET	4.1
1	F	26	ALA	4.0
1	F	182	PHE	4.0
1	E	36	PRO	4.0
1	F	80	GLU	4.0
1	F	59	SER	4.0
1	B	204	ALA	4.0
1	F	67	GLU	4.0
1	F	157	ALA	4.0
1	F	162	LYS	4.0
1	F	161	SER	4.0
1	D	208	LEU	4.0
1	F	33	LEU	4.0
1	F	139	THR	4.0
1	B	210	THR	4.0
1	F	168	THR	4.0
1	E	6	GLN	4.0
1	E	31	THR	3.9
1	F	42	ARG	3.9
1	E	5	GLU	3.9
1	F	131	TYR	3.9
2	L	507	PRO	3.9
1	E	79	ILE	3.9
1	F	66	ILE	3.9
1	F	158	HIS	3.9
1	B	211	LEU	3.9
1	A	208	LEU	3.9
1	F	102	SER	3.9
1	F	152	LYS	3.9
1	F	68	GLN	3.9
1	F	52	VAL	3.9
1	F	60	TRP	3.9
1	C	73	ASP	3.9
1	F	83	ARG	3.9
1	F	231	THR	3.9
1	F	7	LEU	3.8
1	D	118	GLU	3.8
1	E	35	GLU	3.8
1	D	113	SER	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	193	ALA	3.8
1	F	227	ARG	3.8
1	C	213	GLU	3.8
1	F	71	SER	3.8
1	E	9	GLN	3.8
1	F	64	SER	3.8
1	E	7	LEU	3.7
1	F	37	LEU	3.7
1	F	107	TYR	3.7
1	F	8	VAL	3.7
1	F	198	LYS	3.7
1	F	219	SER	3.7
1	E	25	ALA	3.7
1	F	191	GLU	3.7
1	E	213	GLU	3.7
2	G	502	ARG	3.7
1	B	77	LYS	3.6
1	F	224	GLN	3.6
1	F	229	ASN	3.6
1	F	209	ASP	3.6
1	B	67	GLU	3.6
1	F	50	LYS	3.6
1	F	187	GLN	3.6
1	A	212	ASN	3.6
1	C	70	THR	3.6
1	F	113	SER	3.6
1	F	215	SER	3.6
1	F	44	LEU	3.6
1	E	85	TYR	3.6
1	F	125	LYS	3.6
1	D	114	GLU	3.5
1	D	117	TYR	3.5
1	A	76	GLU	3.5
1	A	49	TYR	3.5
1	F	133	TYR	3.5
1	F	193	ALA	3.5
1	C	212	ASN	3.5
1	F	178	ASN	3.5
1	F	88	LYS	3.5
1	E	16	GLN	3.5
1	F	72	ALA	3.5
1	F	155	SER	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	4	ARG	3.5
1	D	2	VAL	3.5
1	F	189	ALA	3.5
1	E	234	THR	3.4
1	F	49	TYR	3.4
1	E	141	GLU	3.4
2	I	502	ARG	3.4
1	B	166	GLN	3.4
1	F	17	ALA	3.4
1	F	144	ALA	3.4
1	A	216	TYR	3.4
1	F	151	GLU	3.4
1	B	208	LEU	3.4
1	B	17	ALA	3.4
1	C	184	TYR	3.4
1	D	116	GLN	3.4
1	D	110	LYS	3.4
1	D	115	THR	3.4
1	F	119	SER	3.4
1	F	180	SER	3.4
1	C	69	LYS	3.3
1	E	69	LYS	3.3
1	F	13	LEU	3.3
1	F	47	VAL	3.3
1	C	215	SER	3.3
1	D	212	ASN	3.3
1	E	12	ARG	3.3
2	I	507	PRO	3.3
1	F	62	VAL	3.3
1	F	147	VAL	3.3
1	A	185	GLU	3.3
1	A	213	GLU	3.3
1	E	11	ALA	3.3
1	E	66	ILE	3.3
1	F	206	ALA	3.3
1	A	187	GLN	3.2
1	C	201	PHE	3.2
1	B	45	LEU	3.2
1	F	146	VAL	3.2
1	F	95	ALA	3.2
1	F	91	LYS	3.2
1	D	166	GLN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	203	ASP	3.2
1	F	202	ASP	3.2
1	B	117	TYR	3.2
1	F	149	SER	3.2
1	B	44	LEU	3.2
1	E	121	VAL	3.2
1	A	6	GLN	3.1
1	A	16	GLN	3.1
1	F	4	ARG	3.1
1	E	214	ASP	3.1
1	F	141	GLU	3.1
1	F	218	ASP	3.1
1	C	202	ASP	3.1
1	E	44	LEU	3.1
1	A	100	VAL	3.1
1	C	200	ALA	3.1
1	F	14	ALA	3.1
1	F	207	GLU	3.1
1	F	54	GLY	3.1
1	E	30	VAL	3.1
1	F	132	ARG	3.1
1	A	160	ILE	3.1
1	E	49	TYR	3.1
1	F	35	GLU	3.1
1	E	101	LEU	3.1
1	F	203	ASP	3.1
1	D	233	TRP	3.1
1	A	42	ARG	3.1
1	A	117	TYR	3.0
1	C	130	TYR	3.0
1	D	165	MET	3.0
1	C	101	LEU	3.0
1	F	228	ASP	3.0
1	B	74	GLY	3.0
1	D	109	ILE	3.0
1	C	67	GLU	3.0
1	A	7	LEU	3.0
1	A	182	PHE	3.0
1	C	194	CYS	3.0
1	F	99	ASP	3.0
1	A	71	SER	3.0
1	E	32	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	24	ALA	3.0
1	F	48	ALA	3.0
1	F	87	GLU	3.0
1	A	123	TYR	3.0
1	A	45	LEU	3.0
2	J	502	ARG	3.0
1	C	99	ASP	3.0
1	D	201	PHE	3.0
1	F	112	CYS	3.0
1	F	28	LYS	3.0
1	C	53	VAL	3.0
1	E	210	THR	3.0
1	E	24	ALA	3.0
1	F	169	HIS	3.0
1	F	106	ASN	3.0
1	E	19	ARG	2.9
1	C	221	LEU	2.9
1	B	52	VAL	2.9
1	D	53	VAL	2.9
1	F	5	GLU	2.9
1	A	135	ALA	2.9
1	F	118	GLU	2.9
1	D	79	ILE	2.9
1	D	168	THR	2.9
1	A	77	LYS	2.9
1	A	153	ALA	2.9
1	E	230	LEU	2.9
1	B	98	GLN	2.9
1	F	116	GLN	2.9
1	B	121	VAL	2.9
2	L	503	ALA	2.9
1	B	214	ASP	2.9
1	E	218	ASP	2.9
1	A	149	SER	2.8
1	F	57	ARG	2.8
1	C	100	VAL	2.8
1	E	37	LEU	2.8
1	E	114	GLU	2.8
1	B	216	TYR	2.8
1	B	140	GLY	2.8
1	A	29	ASN	2.8
1	A	43	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	137	VAL	2.8
1	F	36	PRO	2.8
1	A	70	THR	2.8
1	C	234	THR	2.8
1	E	70	THR	2.8
1	F	153	ALA	2.8
1	D	73	ASP	2.8
1	A	75	ASN	2.8
1	F	39	ASN	2.8
1	A	2	VAL	2.8
1	F	190	PRO	2.8
2	H	507	PRO	2.8
1	B	16	GLN	2.8
1	F	9	GLN	2.8
1	B	12	ARG	2.8
1	C	233	TRP	2.8
1	E	82	VAL	2.8
1	E	81	MET	2.8
1	E	112	CYS	2.8
2	K	504	ILE	2.7
1	B	49	TYR	2.7
1	B	212	ASN	2.7
1	A	189	ALA	2.7
1	D	199	THR	2.7
1	B	185	GLU	2.7
1	F	41	GLU	2.7
1	F	136	GLU	2.7
1	F	3	ASP	2.7
1	D	205	ILE	2.7
1	A	179	TYR	2.7
1	A	17	ALA	2.7
1	D	77	LYS	2.7
1	B	209	ASP	2.7
1	F	21	ASP	2.7
1	A	186	ILE	2.7
1	F	46	SER	2.7
1	A	173	LEU	2.7
1	E	103	LEU	2.7
1	D	200	ALA	2.7
1	B	207	GLU	2.7
1	C	151	GLU	2.7
1	F	166	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	128	GLY	2.7
2	H	504	ILE	2.7
1	C	231	THR	2.7
1	E	185	GLU	2.7
1	F	32	GLU	2.7
1	E	53	VAL	2.6
1	F	148	GLU	2.6
1	A	131	TYR	2.6
1	A	183	TYR	2.6
1	C	204	ALA	2.6
1	E	21	ASP	2.6
1	C	97	CYS	2.6
1	A	37	LEU	2.6
1	A	101	LEU	2.6
1	B	75	ASN	2.6
1	A	53	VAL	2.6
1	B	130	TYR	2.6
1	D	158	HIS	2.6
1	E	99	ASP	2.6
1	A	79	ILE	2.6
1	E	45	LEU	2.6
1	E	34	ASN	2.6
1	B	133	TYR	2.6
1	B	99	ASP	2.6
1	F	56	ARG	2.6
1	F	92	GLU	2.6
1	A	234	THR	2.6
1	D	153	ALA	2.6
1	A	146	VAL	2.5
1	D	11	ALA	2.5
1	D	48	ALA	2.5
1	E	142	LYS	2.5
1	C	49	TYR	2.5
1	A	233	TRP	2.5
1	E	33	LEU	2.5
1	E	211	LEU	2.5
1	B	68	GLN	2.5
1	A	52	VAL	2.5
1	C	8	VAL	2.5
1	D	95	ALA	2.5
1	E	215	SER	2.5
1	C	216	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	74	GLY	2.5
1	D	140	GLY	2.5
1	B	205	ILE	2.5
1	A	232	LEU	2.5
1	D	93	LEU	2.5
1	D	188	ASN	2.5
1	E	43	ASN	2.5
1	F	111	ASN	2.5
1	B	126	MET	2.5
1	D	183	TYR	2.5
1	D	211	LEU	2.5
1	E	78	LYS	2.5
1	D	164	HIS	2.5
1	B	53	VAL	2.5
1	C	137	VAL	2.5
1	C	220	THR	2.5
1	C	166	GLN	2.4
1	E	42	ARG	2.4
1	A	168	THR	2.4
1	D	36	PRO	2.4
1	F	185	GLU	2.4
1	E	110	LYS	2.4
1	C	160	ILE	2.4
2	I	504	ILE	2.4
1	F	188	ASN	2.4
1	E	115	THR	2.4
1	C	35	GLU	2.4
1	C	50	LYS	2.4
1	F	10	LYS	2.4
1	C	134	LEU	2.4
1	F	61	ARG	2.4
1	C	117	TYR	2.4
1	C	39	ASN	2.4
1	F	55	ALA	2.4
1	B	110	LYS	2.4
1	C	198	LYS	2.4
1	F	90	GLU	2.4
1	B	215	SER	2.4
1	B	63	ILE	2.4
1	C	9	GLN	2.4
2	H	506	LEU	2.4
1	D	194	CYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	184	TYR	2.4
1	F	23	MET	2.4
1	C	55	ALA	2.4
1	C	197	ALA	2.4
1	B	163	GLU	2.4
1	E	233	TRP	2.4
1	A	215	SER	2.3
1	A	222	ILE	2.3
1	B	93	LEU	2.3
1	D	63	ILE	2.3
1	E	83	ARG	2.3
1	B	164	HIS	2.3
1	E	208	LEU	2.3
1	B	20	TYR	2.3
1	C	52	VAL	2.3
1	E	212	ASN	2.3
1	A	193	ALA	2.3
1	D	59	SER	2.3
1	C	164	HIS	2.3
1	E	105	ASP	2.3
1	A	96	VAL	2.3
1	A	130	TYR	2.3
1	B	2	VAL	2.3
1	D	49	TYR	2.3
1	E	216	TYR	2.3
1	C	63	ILE	2.3
1	D	160	ILE	2.3
1	E	23	MET	2.3
1	B	194	CYS	2.3
1	D	163	GLU	2.3
1	E	41	GLU	2.3
1	A	167	PRO	2.3
1	B	193	ALA	2.3
1	E	48	ALA	2.3
1	F	34	ASN	2.3
1	B	102	SER	2.3
1	B	66	ILE	2.3
1	B	196	LEU	2.3
1	E	120	LYS	2.3
1	A	118	GLU	2.3
1	F	114	GLU	2.3
1	A	14	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	107	TYR	2.3
1	A	124	LEU	2.2
1	C	93	LEU	2.2
1	C	104	LEU	2.2
1	C	76	GLU	2.2
1	B	82	VAL	2.2
1	A	95	ALA	2.2
1	D	176	ALA	2.2
1	D	184	TYR	2.2
1	C	168	THR	2.2
1	A	128	GLY	2.2
1	B	78	LYS	2.2
1	C	81	MET	2.2
1	F	150	SER	2.2
2	J	504	ILE	2.2
1	D	67	GLU	2.2
1	E	76	GLU	2.2
1	F	40	GLU	2.2
1	C	96	VAL	2.2
1	D	146	VAL	2.2
1	A	106	ASN	2.2
1	C	152	LYS	2.2
1	B	234	THR	2.2
2	G	506	LEU	2.2
1	D	89	ILE	2.2
1	E	40	GLU	2.2
1	B	147	VAL	2.2
1	E	28	LYS	2.2
1	E	193	ALA	2.2
1	B	9	GLN	2.2
1	B	81	MET	2.2
1	E	223	MET	2.2
1	F	16	GLN	2.2
1	A	20	TYR	2.2
1	B	134	LEU	2.2
1	B	230	LEU	2.2
1	C	7	LEU	2.2
1	A	89	ILE	2.2
1	F	38	SER	2.2
1	C	207	GLU	2.2
1	F	22	ASP	2.2
1	F	129	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	167	PRO	2.2
1	A	176	ALA	2.1
1	C	48	ALA	2.1
1	D	98	GLN	2.1
1	E	14	ALA	2.1
2	K	503	ALA	2.1
1	A	159	GLU	2.1
1	A	119	SER	2.1
1	A	180	SER	2.1
1	B	46	SER	2.1
1	D	57	ARG	2.1
1	E	80	GLU	2.1
1	D	161	SER	2.1
1	D	203	ASP	2.1
1	E	65	SER	2.1
1	E	77	LYS	2.1
1	B	96	VAL	2.1
2	I	503	ALA	2.1
1	F	43	ASN	2.1
1	C	103	LEU	2.1
1	B	107	TYR	2.1
1	C	41	GLU	2.1
1	D	76	GLU	2.1
1	E	117	TYR	2.1
1	F	12	ARG	2.1
1	C	3	ASP	2.1
1	B	165	MET	2.1
1	D	52	VAL	2.1
1	B	24	ALA	2.1
1	A	188	ASN	2.1
1	F	29	ASN	2.1
1	A	44	LEU	2.1
1	D	145	THR	2.1
1	C	182	PHE	2.1
1	D	100	VAL	2.1
1	B	104	LEU	2.1
1	C	13	LEU	2.1
1	D	134	LEU	2.1
1	D	20	TYR	2.1
1	B	59	SER	2.1
1	F	65	SER	2.1
1	D	112	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	146	VAL	2.0
1	A	132	ARG	2.0
1	D	55	ALA	2.0
1	A	93	LEU	2.0
1	A	104	LEU	2.0
1	A	211	LEU	2.0
1	A	229	ASN	2.0
1	B	101	LEU	2.0
1	D	43	ASN	2.0
1	D	178	ASN	2.0
1	E	226	LEU	2.0
1	A	18	GLU	2.0
1	A	35	GLU	2.0
1	B	31	THR	2.0
1	E	10	LYS	2.0
1	D	216	TYR	2.0
1	A	97	CYS	2.0
1	C	68	GLN	2.0
1	A	163	GLU	2.0
1	B	50	LYS	2.0
1	B	125	LYS	2.0
1	C	191	GLU	2.0
1	D	196	LEU	2.0
1	B	109	ILE	2.0
1	C	79	ILE	2.0
1	D	66	ILE	2.0
1	D	81	MET	2.0
1	A	219	SER	2.0
1	B	123	TYR	2.0

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. 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
2	SEP	L	505	10/11	0.69	0.18	58,62,65,66	0
2	SEP	J	505	10/11	0.93	0.14	54,56,58,60	0
2	SEP	H	505	10/11	0.94	0.13	56,59,59,61	0
2	SEP	I	505	10/11	0.95	0.14	51,55,60,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SEP	K	505	10/11	0.96	0.10	48,54,57,58	0
2	SEP	G	505	10/11	0.97	0.13	53,58,60,62	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.