



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:23 PM UTC

PDB ID : 9UA8 / pdb_00009ua8
Title : structure of PTP-MEG2 and IFG1R-pY1165/pY1166 peptide complex
Authors : Hu, J.; Liu, H.; Zhang, M.
Deposited on : 2025-03-31
Resolution : 2.00 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

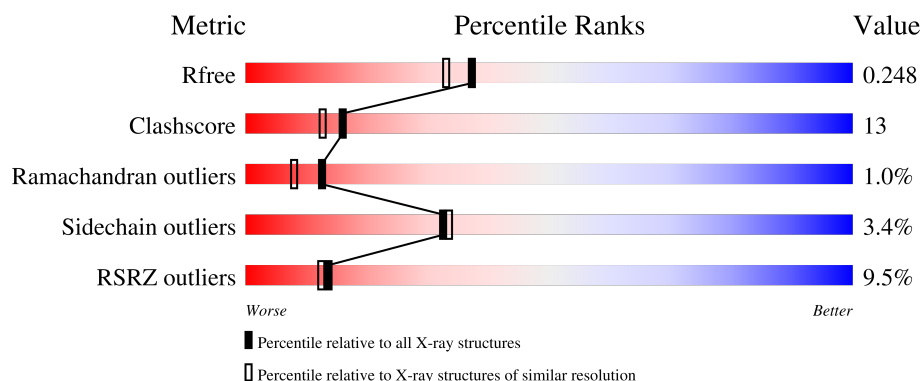
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	305	<div> <div>8%</div> <div>74%</div> <div>19%</div> <div>...</div> </div>
1	B	305	<div> <div>8%</div> <div>76%</div> <div>18%</div> <div>..</div> </div>
1	D	305	<div> <div>10%</div> <div>74%</div> <div>20%</div> <div>..</div> </div>
1	G	305	<div> <div>8%</div> <div>73%</div> <div>22%</div> <div>..</div> </div>
2	C	6	<div> <div>17%</div> <div>33%</div> <div>33%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	6	<div><div></div><div>67%</div><div></div><div>33%</div><div>17%</div><div>33%</div><div>17%</div></div>
2	F	6	<div><div></div><div>33%</div><div>17%</div><div>17%</div><div>33%</div><div>17%</div><div>17%</div></div>
2	H	6	<div><div></div><div>50%</div><div>17%</div><div>67%</div><div>17%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9805 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 Tyrosine-protein phosphatase non-receptor type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	5	0
			2332	1484	400	432	16			
1	B	296	Total	C	N	O	S	0	5	0
			2339	1489	400	434	16			
1	D	296	Total	C	N	O	S	0	5	0
			2344	1492	400	436	16			
1	G	296	Total	C	N	O	S	0	5	0
			2338	1488	399	435	16			

- Molecule 2 is a protein called THR-ASP-PTR-PTR-ARG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	5	Total	C	N	O	P	0	0	0
			58	32	8	16	2			
2	C	4	Total	C	N	O	P	0	0	0
			51	28	7	14	2			
2	E	6	Total	C	N	O	P	0	0	0
			65	37	10	16	2			
2	H	5	Total	C	N	O	P	0	0	0
			58	32	8	16	2			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total	O	0	0
			60	60		
3	F	4	Total	O	0	0
			4	4		
3	B	66	Total	O	0	0
			66	66		
3	C	2	Total	O	0	0
			2	2		

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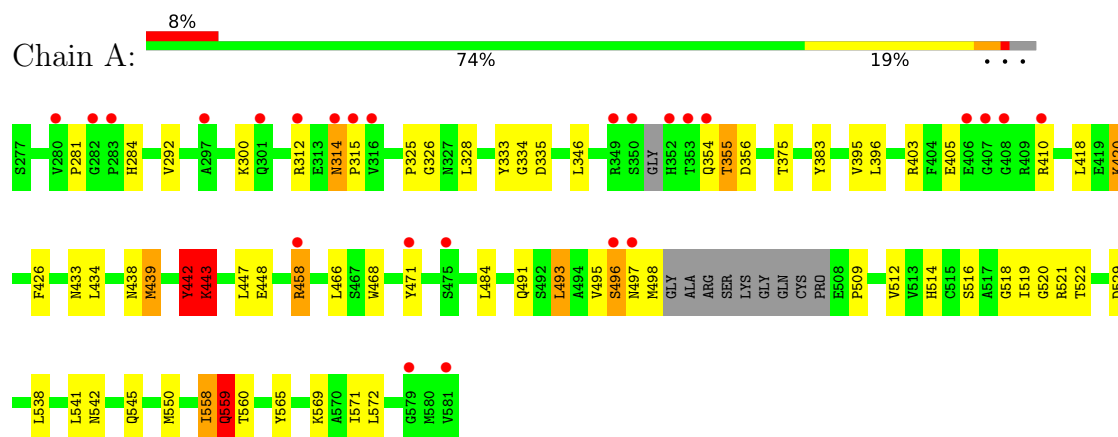
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	42	Total 42	O 42	0	0
3	E	1	Total 1	O 1	0	0
3	G	43	Total 43	O 43	0	0
3	H	2	Total 2	O 2	0	0

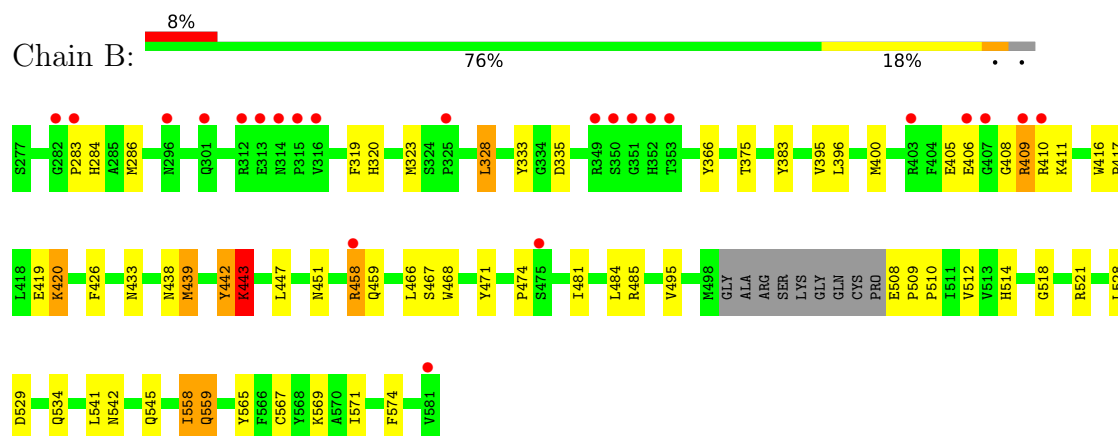
3 Residue-property plots [i](#)

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.

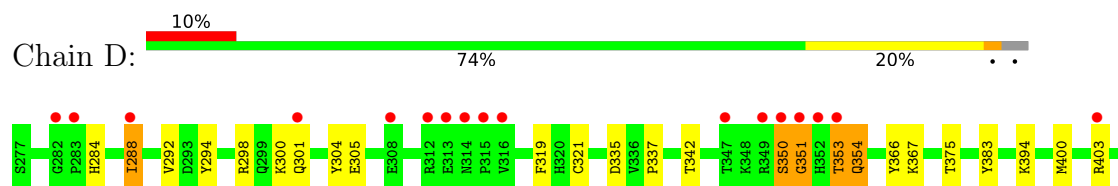
- Molecule 1: Tyrosine-protein phosphatase non-receptor type 9

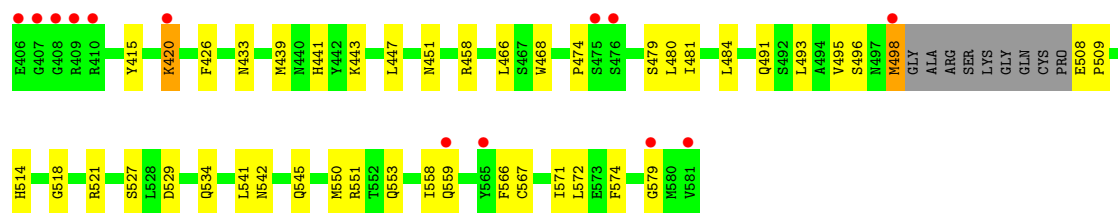


- Molecule 1: Tyrosine-protein phosphatase non-receptor type 9

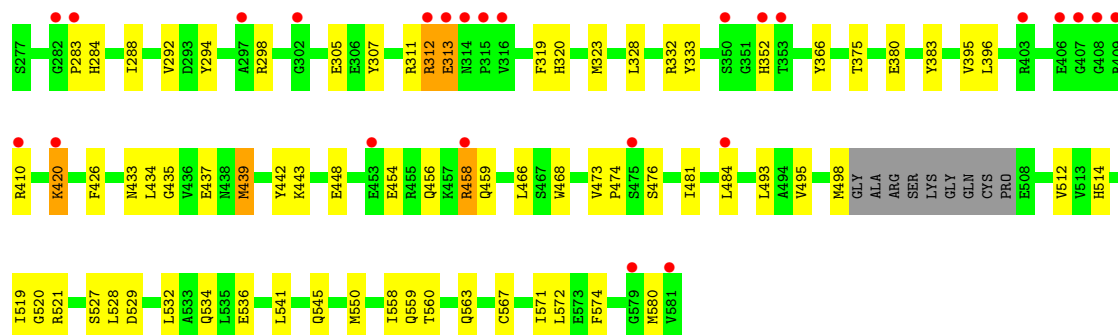
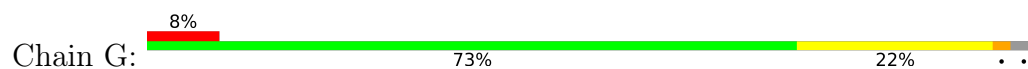


- Molecule 1: Tyrosine-protein phosphatase non-receptor type 9





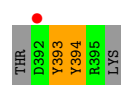
- Molecule 1: Tyrosine-protein phosphatase non-receptor type 9



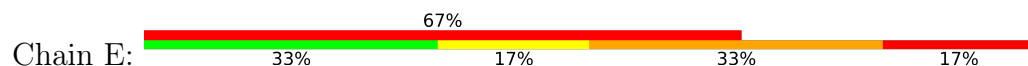
- Molecule 2: THR-ASP-PTR-PTR-ARG



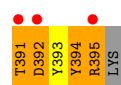
- Molecule 2: THR-ASP-PTR-PTR-ARG



- Molecule 2: THR-ASP-PTR-PTR-ARG



- Molecule 2: THR-ASP-PTR-PTR-ARG



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.29Å 84.71Å 52.67Å 86.03° 94.16° 90.05°	Depositor
Resolution (Å)	36.77 – 2.00 36.77 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (36.77-2.00) 91.9 (36.77-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.6.2_432	Depositor
R, R_{free}	0.217 , 0.254 0.210 , 0.248	Depositor DCC
R_{free} test set	4216 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9805	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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: PTR

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	0.74	6/2408 (0.2%)	0.90	9/3262 (0.3%)
1	B	0.65	3/2416 (0.1%)	0.86	0/3273
1	D	0.56	0/2422	0.82	1/3282 (0.0%)
1	G	0.56	0/2416	0.84	3/3275 (0.1%)
2	C	0.55	0/17	0.56	0/19
2	E	0.63	0/31	0.71	0/37
2	F	0.71	0/24	0.97	0/29
2	H	0.74	0/24	0.61	0/29
All	All	0.63	9/9758 (0.1%)	0.85	13/13206 (0.1%)

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	2
1	B	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	558	ILE	C-O	-7.21	1.15	1.24
1	A	560	THR	C-O	-6.28	1.17	1.24
1	A	442	TYR	C-N	6.25	1.41	1.33
1	B	443	LYS	C-N	-5.89	1.23	1.33
1	A	519	ILE	C-O	-5.82	1.17	1.24
1	A	559	GLN	C-O	-5.58	1.17	1.24
1	A	516	SER	C-O	-5.53	1.17	1.24
1	A	558	ILE	C-O	-5.49	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	442	TYR	C-N	5.18	1.40	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	SER	N-CA-C	-8.66	98.29	110.50
1	A	443	LYS	O-C-N	-8.20	113.76	123.27
1	A	420	LYS	CA-C-N	-6.65	112.02	122.65
1	A	420	LYS	C-N-CA	-6.65	112.02	122.65
1	D	350	SER	N-CA-C	-5.59	105.72	112.54
1	A	420	LYS	N-CA-C	5.46	117.67	111.11
1	G	580	MET	N-CA-C	-5.41	105.99	112.59
1	A	442	TYR	O-C-N	-5.34	117.70	123.42
1	A	314	ASN	CA-C-N	5.31	125.32	119.90
1	A	314	ASN	C-N-CA	5.31	125.32	119.90
1	G	473	VAL	CA-C-N	-5.25	114.54	119.85
1	G	473	VAL	C-N-CA	-5.25	114.54	119.85
1	A	354	GLN	N-CA-C	5.07	119.54	112.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	442	TYR	Mainchain
1	A	443	LYS	Mainchain
1	B	443	LYS	Mainchain

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	2332	0	2213	58	0
1	B	2339	0	2221	61	0
1	D	2344	0	2226	62	0
1	G	2338	0	2216	56	0
2	C	51	0	30	2	0
2	E	65	0	45	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	58	0	37	10	0
2	H	58	0	37	8	0
3	A	60	0	0	3	0
3	B	66	0	0	1	0
3	C	2	0	0	0	0
3	D	42	0	0	2	0
3	E	1	0	0	0	0
3	F	4	0	0	1	0
3	G	43	0	0	5	0
3	H	2	0	0	0	0
All	All	9805	0	9025	247	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 13.

All (247) 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:G:458:ARG:HH21	1:G:458:ARG:HG3	1.12	1.08
1:A:458:ARG:HG3	1:A:458:ARG:HH21	1.21	1.05
1:B:458:ARG:HH21	1:B:458:ARG:HG3	1.21	1.04
1:D:354:GLN:HA	1:D:354:GLN:NE2	1.71	1.03
1:A:334:GLY:H	2:F:392:ASP:HB3	1.25	1.00
1:B:406:GLU:O	1:B:409:ARG:CG	2.10	0.98
1:D:354:GLN:HA	1:D:354:GLN:HE21	1.26	0.94
1:G:332:ARG:HH22	1:G:410:ARG:HH12	1.14	0.93
1:A:325:PRO:HA	3:A:601:HOH:O	1.70	0.91
1:B:406:GLU:O	1:B:409:ARG:HG3	1.72	0.90
1:A:420:LYS:O	1:A:433:ASN:O	1.91	0.89
1:G:420:LYS:O	1:G:433:ASN:O	1.91	0.89
1:A:334:GLY:H	2:F:392:ASP:CB	1.86	0.87
1:D:420:LYS:O	1:D:433:ASN:O	1.93	0.87
1:B:284:HIS:H	1:B:545:GLN:HE22	1.22	0.84
1:B:458:ARG:HH21	1:B:458:ARG:CG	1.91	0.82
1:A:471:TYR:HD1	1:A:559:GLN:HE22	1.26	0.81
2:E:395:ARG:HH11	2:E:395:ARG:CG	1.93	0.81
1:A:284:HIS:H	1:A:545:GLN:HE22	1.28	0.81
1:B:485:ARG:HH21	1:B:574:PHE:HE1	1.31	0.77
1:G:458:ARG:HH21	1:G:458:ARG:CG	1.93	0.77
1:A:458:ARG:HH21	1:A:458:ARG:CG	1.98	0.77
1:A:326:GLY:N	3:A:601:HOH:O	2.11	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:HIS:H	1:D:545:GLN:HE22	1.33	0.76
1:A:496:SER:O	1:A:497:ASN:HB2	1.85	0.75
1:G:332:ARG:HH22	1:G:410:ARG:NH1	1.86	0.74
1:A:471:TYR:HD1	1:A:559:GLN:NE2	1.85	0.74
1:B:420:LYS:O	1:B:433:ASN:O	2.07	0.73
1:G:284:HIS:H	1:G:545:GLN:HE22	1.33	0.73
1:G:458:ARG:HG3	1:G:458:ARG:NH2	1.91	0.72
1:D:354:GLN:HE21	1:D:354:GLN:CA	1.98	0.72
1:G:567:CYS:O	1:G:571[A]:ILE:HG12	1.90	0.71
1:A:334:GLY:N	2:F:392:ASP:HB3	2.04	0.71
1:B:458:ARG:HG3	1:B:458:ARG:NH2	2.02	0.69
2:F:391:THR:N	3:F:401:HOH:O	2.24	0.68
1:A:541:LEU:CD1	1:A:571[B]:ILE:HD13	2.23	0.68
1:A:565:TYR:OH	1:A:569[A]:LYS:HE2	1.93	0.68
2:H:391:THR:O	2:H:392:ASP:HB2	1.93	0.68
1:A:335:ASP:CG	2:F:393:PTR:HA	2.18	0.67
1:B:406:GLU:O	1:B:409:ARG:HG2	1.93	0.67
1:B:420:LYS:O	1:B:433:ASN:HB3	1.96	0.65
1:G:437:GLU:OE2	3:G:602:HOH:O	2.14	0.65
1:B:567:CYS:O	1:B:571[A]:ILE:HG12	1.96	0.65
1:A:405:GLU:HG2	1:A:410:ARG:HA	1.79	0.65
1:D:300:LYS:HE2	1:D:304:TYR:OH	1.97	0.65
1:B:565:TYR:OH	1:B:569[A]:LYS:HE2	1.97	0.64
1:G:528:LEU:HD12	1:G:571[A]:ILE:HD11	1.79	0.64
1:G:560:THR:OG1	1:G:563:GLN:HG3	1.98	0.64
1:D:551:ARG:HH22	2:E:396:LYS:HZ1	1.44	0.64
1:G:495:VAL:O	1:G:498:MET:HB2	1.98	0.64
1:G:332:ARG:NH2	1:G:410:ARG:HH12	1.93	0.63
1:A:284:HIS:HB2	1:A:545:GLN:NE2	2.14	0.63
1:D:491:GLN:O	1:D:495:VAL:HG23	1.99	0.63
1:G:380:GLU:OE2	3:G:603:HOH:O	2.15	0.63
1:B:335:ASP:HB3	2:C:393:PTR:HD1	1.81	0.63
1:A:396:LEU:HD23	1:A:458:ARG:HD3	1.81	0.63
2:E:395:ARG:HH11	2:E:395:ARG:HG2	1.65	0.62
1:D:301:GLN:O	1:D:305:GLU:HG3	2.00	0.61
1:A:439:MET:HG2	1:A:442:TYR:CZ	2.35	0.61
1:A:458:ARG:HG3	1:A:458:ARG:NH2	2.02	0.61
1:A:484:LEU:HD21	1:A:529:ASP:HA	1.83	0.60
1:D:468:TRP:CE2	1:D:474:PRO:HD3	2.36	0.60
2:E:395:ARG:HH11	2:E:395:ARG:HG3	1.67	0.60
1:G:493:LEU:HD23	1:G:493:LEU:C	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:394:PTR:C	2:H:395:ARG:HD3	2.32	0.60
1:A:496:SER:O	1:A:497:ASN:CB	2.48	0.60
1:B:541:LEU:CD1	1:B:571[B]:ILE:HD13	2.32	0.59
1:A:292:VAL:HG22	1:A:572:LEU:HD22	1.84	0.59
1:B:541:LEU:HD13	1:B:571[B]:ILE:HD13	1.85	0.59
1:B:383:TYR:HB3	1:B:426:PHE:CE1	2.38	0.58
1:D:292:VAL:HG22	1:D:572:LEU:HD22	1.86	0.58
1:G:541:LEU:CD1	1:G:571[B]:ILE:HD13	2.33	0.58
1:D:579:GLY:HA3	1:G:352:HIS:CE1	2.39	0.58
1:G:319:PHE:HB2	1:G:323:MET:HE2	1.86	0.57
1:G:443:LYS:HG3	1:G:466:LEU:HD11	1.86	0.57
1:B:528:LEU:HD12	1:B:571[A]:ILE:HD11	1.85	0.57
1:D:350:SER:O	1:D:351:GLY:O	2.23	0.57
1:A:493:LEU:O	1:A:496:SER:O	2.23	0.56
1:G:307:TYR:CE2	1:G:311:ARG:HD2	2.40	0.56
1:G:410:ARG:NH2	3:G:606:HOH:O	2.37	0.56
1:D:298:ARG:HH21	1:D:298:ARG:HG3	1.70	0.56
1:B:485:ARG:NH1	3:B:602:HOH:O	2.39	0.56
2:E:394:PTR:C	2:E:395:ARG:HG3	2.36	0.56
1:A:484:LEU:HD11	1:A:529:ASP:OD1	2.06	0.56
1:G:292:VAL:HG22	1:G:572:LEU:HD22	1.88	0.56
1:G:439:MET:HG2	1:G:442:TYR:CZ	2.41	0.55
1:B:320:HIS:HB3	1:G:320:HIS:O	2.07	0.55
1:D:443:LYS:HG3	1:D:466:LEU:HD11	1.88	0.54
1:D:559:GLN:OE1	2:E:396:LYS:HB2	2.07	0.54
1:D:567:CYS:O	1:D:571[A]:ILE:HG12	2.08	0.54
1:B:468:TRP:CE2	1:B:521:ARG:HG2	2.43	0.54
1:D:551:ARG:HH22	2:E:396:LYS:NZ	2.05	0.54
1:D:294:TYR:CE1	1:D:298:ARG:CZ	2.91	0.54
1:G:454:GLU:O	1:G:456:GLN:HG3	2.08	0.53
1:D:474:PRO:HG2	1:D:566:PHE:CZ	2.43	0.53
1:A:284:HIS:N	1:A:545:GLN:HE22	2.03	0.53
1:B:366:TYR:CE1	1:B:534:GLN:HG3	2.43	0.53
1:G:283:PRO:HD2	1:G:545:GLN:NE2	2.24	0.53
1:B:284:HIS:HB2	1:B:545:GLN:NE2	2.23	0.53
1:G:420:LYS:HG2	1:G:435:GLY:HA2	1.90	0.52
1:A:383:TYR:HB3	1:A:426:PHE:CE1	2.44	0.52
1:B:439:MET:HG2	1:B:442:TYR:CZ	2.45	0.52
1:D:298:ARG:HG3	1:D:298:ARG:NH2	2.24	0.52
1:G:332:ARG:HH12	1:G:410:ARG:HH11	1.56	0.52
1:A:458:ARG:CG	1:A:458:ARG:NH2	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:383:TYR:HB3	1:G:426:PHE:CE1	2.45	0.51
1:D:541:LEU:CD1	1:D:571[B]:ILE:HD13	2.40	0.51
1:G:458:ARG:CG	1:G:458:ARG:NH2	2.58	0.51
1:G:395:VAL:HG21	1:G:512:VAL:HG23	1.92	0.51
1:B:485:ARG:NH2	1:B:574:PHE:HE1	2.02	0.51
1:A:468:TRP:CE2	1:A:521:ARG:HG2	2.46	0.50
1:B:319:PHE:HB2	1:B:323:MET:HE2	1.93	0.50
1:D:468:TRP:CE2	1:D:521:ARG:HG2	2.46	0.50
1:A:300:LYS:HG3	1:A:565:TYR:CZ	2.47	0.50
1:B:458:ARG:HD2	1:B:459:GLN:O	2.12	0.50
1:G:468:TRP:CE2	1:G:474:PRO:HD3	2.47	0.49
1:G:458:ARG:HD2	1:G:459:GLN:O	2.12	0.49
1:B:468:TRP:CE2	1:B:474:PRO:HD3	2.47	0.49
1:G:332:ARG:O	2:H:391:THR:HG23	2.11	0.49
2:E:395:ARG:CG	2:E:395:ARG:NH1	2.64	0.49
1:G:527:SER:N	1:G:550:MET:HE1	2.28	0.49
1:A:312:ARG:NH1	1:A:312:ARG:HB2	2.27	0.49
1:B:438:ASN:HD21	1:B:443:LYS:HE3	1.77	0.49
1:G:294:TYR:CE1	1:G:298:ARG:CZ	2.95	0.49
1:A:471:TYR:CD1	1:A:559:GLN:NE2	2.75	0.49
1:A:433:ASN:HA	1:A:447:LEU:HD23	1.95	0.48
1:G:396:LEU:HD23	1:G:458:ARG:HD3	1.95	0.48
1:G:484:LEU:HD11	1:G:529:ASP:OD1	2.14	0.48
1:G:366:TYR:CE1	1:G:534:GLN:HG3	2.48	0.48
1:G:468:TRP:CE2	1:G:521:ARG:HG2	2.48	0.48
1:G:410:ARG:CZ	3:G:606:HOH:O	2.61	0.48
1:G:434:LEU:HD11	1:G:448:GLU:HB2	1.96	0.48
2:H:391:THR:O	2:H:391:THR:HG22	2.14	0.48
1:G:333:TYR:CG	2:H:394:PTR:HB3	2.49	0.48
1:D:400:MET:HG3	1:D:514:HIS:CE1	2.49	0.48
1:D:542:ASN:CG	1:D:545:GLN:HG3	2.39	0.47
2:H:391:THR:O	2:H:392:ASP:CB	2.61	0.47
1:A:518:GLY:HA2	1:A:522:THR:OG1	2.13	0.47
1:B:542:ASN:OD1	1:B:545:GLN:HG3	2.14	0.47
1:A:471:TYR:HE1	2:F:394:PTR:O	1.97	0.47
1:B:395:VAL:HG21	1:B:512:VAL:HG23	1.95	0.47
1:D:541:LEU:HD12	1:D:571[B]:ILE:HD13	1.96	0.47
1:G:332:ARG:HG3	2:H:391:THR:HG21	1.97	0.47
1:D:284:HIS:HB2	1:D:545:GLN:NE2	2.30	0.47
1:D:284:HIS:N	1:D:545:GLN:HE22	2.08	0.47
1:B:283:PRO:HD2	1:B:545:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:GLN:NE2	3:D:606:HOH:O	2.48	0.47
1:B:284:HIS:N	1:B:545:GLN:HE22	2.00	0.47
1:B:458:ARG:CG	1:B:458:ARG:NH2	2.60	0.47
1:D:542:ASN:OD1	1:D:545:GLN:HG3	2.14	0.47
1:B:528:LEU:HD12	1:B:571[A]:ILE:CD1	2.44	0.47
1:G:332:ARG:O	2:H:391:THR:CG2	2.62	0.47
1:B:409:ARG:NH1	1:B:411:LYS:NZ	2.63	0.47
1:G:519:ILE:HG13	1:G:520:GLY:N	2.30	0.47
1:A:335:ASP:HB3	2:F:393:PTR:HD1	1.97	0.46
1:G:312:ARG:O	1:G:313:GLU:O	2.32	0.46
1:D:484:LEU:HD21	1:D:529:ASP:HA	1.96	0.46
1:D:496:SER:C	1:D:498:MET:H	2.24	0.46
1:B:405:GLU:OE1	1:B:408:GLY:HA2	2.15	0.46
1:B:416:TRP:HB2	1:B:417:PRO:HD2	1.97	0.46
1:B:484:LEU:HD21	1:B:529:ASP:HA	1.98	0.46
1:D:527:SER:N	1:D:550:MET:HE1	2.31	0.46
1:A:346:LEU:O	1:A:356:ASP:HB2	2.16	0.45
1:D:366:TYR:CE1	1:D:534:GLN:HG3	2.50	0.45
1:D:342:THR:HG21	1:D:553:GLN:HA	1.99	0.45
1:A:471:TYR:CE1	2:F:394:PTR:O	2.69	0.45
1:A:312:ARG:HB2	1:A:312:ARG:HH11	1.82	0.45
1:A:491:GLN:O	1:A:495:VAL:HG23	2.17	0.45
1:A:498:MET:HE1	1:A:509:PRO:HG3	1.97	0.45
1:D:498:MET:HE1	1:D:509:PRO:HG3	1.99	0.45
1:A:395:VAL:HG21	1:A:512:VAL:HG23	1.97	0.45
1:B:471:TYR:HD1	1:B:559:GLN:HE22	1.56	0.45
1:D:441:HIS:CD2	1:D:479[B]:SER:HB2	2.52	0.45
1:G:484:LEU:HD11	1:G:529:ASP:CG	2.42	0.45
1:A:375:THR:O	1:A:518:GLY:HA3	2.17	0.44
1:B:419:GLU:O	1:B:420:LYS:C	2.60	0.44
1:D:353:THR:HG23	1:D:353:THR:O	2.17	0.44
1:G:307:TYR:CE2	1:G:311:ARG:CD	3.00	0.44
1:D:508:GLU:HA	1:D:509:PRO:HD3	1.90	0.44
1:G:288:ILE:HD12	1:G:288:ILE:HA	1.78	0.44
1:G:458:ARG:NH2	3:G:601:HOH:O	2.09	0.44
1:B:484:LEU:HD11	1:B:529:ASP:CG	2.43	0.44
1:B:495:VAL:HG21	1:B:508:GLU:HG3	1.99	0.44
1:D:354:GLN:NE2	1:D:354:GLN:CA	2.50	0.44
1:B:438:ASN:ND2	1:B:443:LYS:HE3	2.33	0.44
1:D:481:ILE:CD1	1:D:574:PHE:HB2	2.47	0.44
2:E:395:ARG:O	2:E:396:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:PRO:CA	3:A:601:HOH:O	2.47	0.43
1:A:333:TYR:CG	2:F:394:PTR:HB3	2.53	0.43
1:B:320:HIS:O	1:G:320:HIS:HB3	2.18	0.43
1:B:406:GLU:O	1:B:409:ARG:CD	2.65	0.43
1:D:288:ILE:HA	1:D:288:ILE:HD13	1.69	0.43
1:D:495:VAL:O	1:D:498:MET:HB3	2.17	0.43
1:A:281:PRO:HG3	1:A:538:LEU:HD12	1.99	0.43
1:B:443:LYS:HG3	1:B:466:LEU:HD11	1.99	0.43
1:B:542:ASN:CG	1:B:545:GLN:HG3	2.43	0.43
1:B:565:TYR:OH	1:B:569[B]:LYS:HE3	2.19	0.43
1:D:551:ARG:HH22	2:E:396:LYS:CE	2.30	0.43
1:D:474:PRO:HG3	1:D:480:LEU:HD22	2.01	0.43
1:B:333:TYR:CG	2:C:394:PTR:HB3	2.53	0.43
1:B:567:CYS:O	1:B:571[B]:ILE:HG13	2.19	0.43
1:A:434:LEU:HD11	1:A:448:GLU:HB2	2.01	0.42
1:B:328:LEU:HD12	1:B:328:LEU:HA	1.84	0.42
1:B:375:THR:O	1:B:518:GLY:HA3	2.19	0.42
1:D:394:LYS:HA	1:D:458:ARG:NH2	2.34	0.42
1:D:420:LYS:O	1:D:433:ASN:HB3	2.19	0.42
1:D:366:TYR:OH	1:D:367:LYS:HE3	2.18	0.42
1:D:551:ARG:HH12	2:E:396:LYS:NZ	2.17	0.42
1:G:375:THR:O	1:G:514:HIS:HB2	2.20	0.42
1:A:314:ASN:HA	1:A:315:PRO:HD3	1.89	0.42
1:A:375:THR:O	1:A:514:HIS:HB2	2.20	0.42
1:A:418:LEU:HD23	1:A:418:LEU:HA	1.90	0.42
1:A:438:ASN:ND2	1:A:443:LYS:HE3	2.33	0.42
1:B:375:THR:O	1:B:514:HIS:HB2	2.20	0.41
1:D:321[B]:CYS:HB2	3:D:609:HOH:O	2.20	0.41
1:B:481:ILE:CD1	1:B:574:PHE:HB2	2.50	0.41
1:D:481:ILE:HD13	1:D:574:PHE:HB2	2.02	0.41
1:G:493:LEU:C	1:G:493:LEU:CD2	2.93	0.41
1:B:433:ASN:HA	1:B:447:LEU:HD23	2.01	0.41
1:D:383:TYR:HB3	1:D:426:PHE:CE1	2.54	0.41
1:D:433:ASN:HA	1:D:447:LEU:HD23	2.01	0.41
1:G:481:ILE:CD1	1:G:574:PHE:HB2	2.51	0.41
1:B:409:ARG:NH1	1:B:411:LYS:HZ1	2.18	0.41
1:B:451:ASN:C	1:B:451:ASN:OD1	2.64	0.41
1:A:550:MET:HE3	1:A:550:MET:HB2	1.93	0.41
1:D:350:SER:C	1:D:351:GLY:O	2.63	0.41
1:D:484:LEU:HD11	1:D:529:ASP:CG	2.46	0.41
1:A:542:ASN:CG	1:A:545:GLN:HG3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:TYR:CE1	1:D:415:TYR:HB3	2.56	0.41
1:D:550:MET:HE3	1:D:550:MET:HB2	1.94	0.41
1:A:520:GLY:HA2	1:A:559:GLN:HB2	2.03	0.40
1:D:451:ASN:OD1	1:D:451:ASN:C	2.65	0.40
1:D:551:ARG:NH2	2:E:396:LYS:HZ1	2.14	0.40
1:B:400:MET:HG3	1:B:514:HIS:CE1	2.56	0.40
1:D:375:THR:O	1:D:518:GLY:HA3	2.21	0.40
2:E:393:PTR:O1P	2:E:393:PTR:CE1	2.70	0.40
2:E:395:ARG:HG3	2:E:395:ARG:NH1	2.33	0.40
1:A:443:LYS:HG3	1:A:466:LEU:HD11	2.03	0.40
1:B:286:MET:HE3	1:B:286:MET:HB2	1.91	0.40
1:D:319:PHE:HB3	1:D:337:PRO:HB2	2.03	0.40
1:D:335:ASP:OD2	2:E:395:ARG:N	2.52	0.40
1:A:541:LEU:HD13	1:A:571[B]:ILE:HD13	2.00	0.40
1:A:559:GLN:HG3	2:F:394:PTR:HE2	2.04	0.40
1:B:396:LEU:HD23	1:B:458:ARG:HD3	2.04	0.40
1:B:509:PRO:HA	1:B:510:PRO:HD3	2.00	0.40
1:G:532:LEU:O	1:G:536:GLU:HG3	2.20	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	294/305 (96%)	279 (95%)	13 (4%)	2 (1%)	18	14
1	B	297/305 (97%)	287 (97%)	8 (3%)	2 (1%)	18	14
1	D	297/305 (97%)	284 (96%)	11 (4%)	2 (1%)	18	14
1	G	297/305 (97%)	284 (96%)	10 (3%)	3 (1%)	12	8
2	E	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
2	F	1/6 (17%)	0	0	1 (100%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	1/6 (17%)	0	0	1 (100%)	0	0
All	All	1189/1238 (96%)	1135 (96%)	42 (4%)	12 (1%)	12	8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	420	LYS
2	E	395	ARG
1	G	313	GLU
2	H	392	ASP
1	A	355	THR
2	F	392	ASP
1	D	351	GLY
1	G	312	ARG
1	A	558	ILE
1	B	558	ILE
1	D	558	ILE
1	G	558	ILE

5.3.2 Protein sidechains [i](#)

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	246/270 (91%)	239 (97%)	7 (3%)	38	41
1	B	246/270 (91%)	239 (97%)	7 (3%)	38	41
1	D	248/270 (92%)	240 (97%)	8 (3%)	34	35
1	G	247/270 (92%)	240 (97%)	7 (3%)	38	41
2	C	2/4 (50%)	2 (100%)	0	100	100
2	E	3/4 (75%)	2 (67%)	1 (33%)	0	0
2	F	3/4 (75%)	2 (67%)	1 (33%)	0	0
2	H	3/4 (75%)	1 (33%)	2 (67%)	0	0
All	All	998/1096 (91%)	965 (97%)	33 (3%)	32	34

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	LEU
1	A	355	THR
1	A	403	ARG
1	A	439	MET
1	A	458	ARG
1	A	493	LEU
1	A	559	GLN
2	F	392	ASP
1	B	328	LEU
1	B	409	ARG
1	B	410	ARG
1	B	439	MET
1	B	458	ARG
1	B	467	SER
1	B	559	GLN
1	D	288	ILE
1	D	353	THR
1	D	354	GLN
1	D	403	ARG
1	D	420	LYS
1	D	439	MET
1	D	493	LEU
1	D	498	MET
2	E	395	ARG
1	G	305	GLU
1	G	328	LEU
1	G	420	LYS
1	G	439	MET
1	G	458	ARG
1	G	476	SER
1	G	559	GLN
2	H	391	THR
2	H	395	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	438	ASN
1	A	489	ASN
1	A	545	GLN
1	A	559	GLN

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Mol	Chain	Res	Type
1	B	438	ASN
1	B	489	ASN
1	B	545	GLN
1	B	559	GLN
1	D	354	GLN
1	D	489	ASN
1	D	545	GLN
1	G	352	HIS
1	G	489	ASN
1	G	545	GLN
1	G	559	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	PTR	C	393	2	15,16,17	1.94	1 (6%)	17,22,24	0.62	0
2	PTR	H	394	2	15,16,17	2.07	1 (6%)	17,22,24	0.79	0
2	PTR	E	394	2	15,16,17	2.07	1 (6%)	17,22,24	0.67	0
2	PTR	E	393	2	15,16,17	1.97	2 (13%)	17,22,24	0.63	0
2	PTR	H	393	2	15,16,17	1.99	1 (6%)	17,22,24	0.55	0
2	PTR	F	393	2	15,16,17	1.96	1 (6%)	17,22,24	0.60	0
2	PTR	F	394	2	15,16,17	2.07	1 (6%)	17,22,24	0.64	0
2	PTR	C	394	2	15,16,17	1.93	1 (6%)	17,22,24	0.71	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	PTR	C	393	2	-	0/10/11/13	0/1/1/1
2	PTR	H	394	2	-	0/10/11/13	0/1/1/1
2	PTR	E	394	2	-	1/10/11/13	0/1/1/1
2	PTR	E	393	2	-	1/10/11/13	0/1/1/1
2	PTR	H	393	2	-	2/10/11/13	0/1/1/1
2	PTR	F	393	2	-	4/10/11/13	0/1/1/1
2	PTR	F	394	2	-	0/10/11/13	0/1/1/1
2	PTR	C	394	2	-	0/10/11/13	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	394	PTR	OH-CZ	-7.83	1.23	1.40
2	E	394	PTR	OH-CZ	-7.79	1.23	1.40
2	F	394	PTR	OH-CZ	-7.63	1.23	1.40
2	H	393	PTR	OH-CZ	-7.42	1.24	1.40
2	F	393	PTR	OH-CZ	-7.31	1.24	1.40
2	C	393	PTR	OH-CZ	-7.22	1.24	1.40
2	C	394	PTR	OH-CZ	-7.22	1.24	1.40
2	E	393	PTR	OH-CZ	-7.18	1.24	1.40
2	E	393	PTR	P-OH	2.15	1.63	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	393	PTR	O-C-CA-CB
2	E	394	PTR	O-C-CA-CB
2	E	393	PTR	N-CA-CB-CG
2	H	393	PTR	CA-CB-CG-CD1
2	H	393	PTR	CA-CB-CG-CD2
2	F	393	PTR	CA-CB-CG-CD1
2	F	393	PTR	CA-CB-CG-CD2
2	F	393	PTR	CZ-OH-P-O2P

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	393	PTR	1	0
2	H	394	PTR	2	0
2	E	394	PTR	1	0
2	E	393	PTR	1	0
2	F	393	PTR	2	0
2	F	394	PTR	4	0
2	C	394	PTR	1	0

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	295/305 (96%)	0.37	25 (8%) 16 15	12, 22, 50, 64	5 (1%)
1	B	296/305 (97%)	0.41	23 (7%) 19 18	12, 23, 52, 69	5 (1%)
1	D	296/305 (97%)	0.57	30 (10%) 12 11	12, 25, 55, 69	5 (1%)
1	G	296/305 (97%)	0.55	25 (8%) 17 15	12, 25, 53, 81	5 (1%)
2	C	2/6 (33%)	1.87	1 (50%) 0 1	38, 38, 38, 60	0
2	E	4/6 (66%)	4.28	4 (100%) 0 0	48, 65, 67, 76	0
2	F	3/6 (50%)	2.98	2 (66%) 0 0	37, 37, 62, 70	0
2	H	3/6 (50%)	3.64	3 (100%) 0 0	56, 56, 63, 65	0
All	All	1195/1244 (96%)	0.50	113 (9%) 14 12	12, 24, 54, 81	20 (1%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	391	THR	8.1
1	G	316	VAL	6.1
1	D	316	VAL	5.8
1	G	314	ASN	5.6
1	A	316	VAL	5.6
1	B	316	VAL	5.5
1	G	407	GLY	5.2
1	G	315	PRO	4.9
1	A	352	HIS	4.8
1	A	581	VAL	4.7
1	B	581	VAL	4.6
2	H	391	THR	4.5
1	D	351	GLY	4.3
1	A	353	THR	4.3
2	F	391	THR	4.2
1	D	581	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	315	PRO	4.1
1	D	406	GLU	4.0
1	G	408	GLY	4.0
1	D	410	ARG	3.9
1	G	410	ARG	3.9
1	B	314	ASN	3.9
2	H	395	ARG	3.8
1	G	406	GLU	3.8
1	A	350	SER	3.8
1	B	410	ARG	3.8
1	G	581	VAL	3.7
1	G	475	SER	3.6
1	B	313	GLU	3.6
1	A	354	GLN	3.6
1	D	314	ASN	3.6
1	D	282	GLY	3.5
1	G	353	THR	3.4
2	E	395	ARG	3.4
1	D	350	SER	3.3
1	G	352	HIS	3.3
1	D	312	ARG	3.3
1	G	313	GLU	3.3
1	B	409	ARG	3.3
1	A	410	ARG	3.2
1	B	353	THR	3.2
2	F	392	ASP	3.2
1	D	352	HIS	3.1
1	B	352	HIS	3.1
1	B	407	GLY	3.1
1	A	406	GLU	3.0
1	A	407	GLY	3.0
1	D	315	PRO	3.0
1	G	282	GLY	3.0
1	A	315	PRO	3.0
1	D	313	GLU	3.0
2	E	396	LYS	3.0
1	B	475	SER	2.9
1	B	350	SER	2.9
1	D	408	GLY	2.9
1	B	458	ARG	2.8
1	B	296	ASN	2.8
1	D	475	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	312	ARG	2.8
1	G	312	ARG	2.7
1	A	283	PRO	2.7
1	G	420	LYS	2.7
1	A	282	GLY	2.7
1	D	579	GLY	2.7
1	A	297	ALA	2.6
1	A	408	GLY	2.6
1	G	297	ALA	2.6
2	E	392	ASP	2.6
1	D	349	ARG	2.6
1	D	409	ARG	2.6
1	B	406	GLU	2.6
1	G	458	ARG	2.6
1	D	301	GLN	2.6
1	D	476	SER	2.6
1	D	407	GLY	2.6
1	D	353	THR	2.6
2	H	392	ASP	2.5
1	B	282	GLY	2.5
1	A	475	SER	2.5
1	B	312	ARG	2.5
1	G	350	SER	2.5
1	D	283	PRO	2.5
1	B	301	GLN	2.5
2	C	392	ASP	2.4
1	B	403	ARG	2.4
1	G	453	GLU	2.4
1	A	458	ARG	2.4
1	D	498	MET	2.4
1	G	484	LEU	2.3
1	D	347	THR	2.3
1	A	497	ASN	2.3
1	B	283	PRO	2.3
1	B	349	ARG	2.3
1	A	471	TYR	2.3
1	G	403	ARG	2.3
1	D	288	ILE	2.3
1	D	559	GLN	2.3
1	A	349	ARG	2.2
1	G	302	GLY	2.2
1	A	280	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	314	ASN	2.2
1	D	420	LYS	2.2
1	A	496	SER	2.2
1	D	403	ARG	2.2
1	D	308	GLU	2.1
1	A	579	GLY	2.1
1	B	351	GLY	2.1
1	A	301	GLN	2.1
1	G	283	PRO	2.0
1	G	409	ARG	2.0
1	G	579	GLY	2.0
1	D	565	TYR	2.0
1	B	325	PRO	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. 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(Å ²)	Q<0.9
2	PTR	E	393	16/17	0.52	0.21	59,79,103,132	0
2	PTR	H	393	16/17	0.61	0.20	42,69,84,109	0
2	PTR	F	393	16/17	0.64	0.21	50,71,92,110	0
2	PTR	C	393	16/17	0.69	0.20	44,71,92,110	0
2	PTR	E	394	16/17	0.97	0.07	17,22,38,40	0
2	PTR	C	394	16/17	0.98	0.07	13,19,33,34	0
2	PTR	F	394	16/17	0.98	0.06	11,18,33,36	0
2	PTR	H	394	16/17	0.98	0.06	15,22,33,37	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.