Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 02:54 AM EST

PDB ID	:	8V08
Title	:	Crystal structure of human PLD4 co-crystallized with 5'Pi-ssDNA
Authors	:	Yuan, M.; Wilson, I.A.
Deposited on	:	2023-11-17
Resolution	:	3.00 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 (i) 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 (1)) were used in the production of this report:

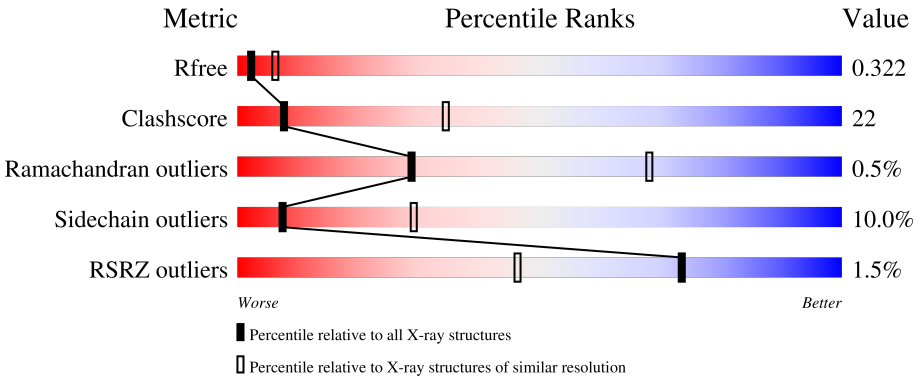
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	488	% 45% 32% · 20%
2	B	488	% 41% 35% · 20%
3	C	3	33% 67%
3	D	3	33% 100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6232 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 5'-3' exonuclease PLD4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	392	3065	1954	536	562	1	12	0	1	0

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	HIS	-	expression tag	UNP Q96BZ4
A	20	HIS	-	expression tag	UNP Q96BZ4
A	21	HIS	-	expression tag	UNP Q96BZ4
A	22	HIS	-	expression tag	UNP Q96BZ4
A	23	HIS	-	expression tag	UNP Q96BZ4
A	24	HIS	-	expression tag	UNP Q96BZ4
A	25	GLY	-	expression tag	UNP Q96BZ4
A	26	PRO	-	expression tag	UNP Q96BZ4
A	27	LEU	-	expression tag	UNP Q96BZ4
A	28	VAL	-	expression tag	UNP Q96BZ4
A	29	ASP	-	expression tag	UNP Q96BZ4
A	30	VAL	-	expression tag	UNP Q96BZ4
A	31	ALA	-	expression tag	UNP Q96BZ4
A	32	SER	-	expression tag	UNP Q96BZ4
A	33	ASN	-	expression tag	UNP Q96BZ4
A	34	GLU	-	expression tag	UNP Q96BZ4
A	35	GLN	-	expression tag	UNP Q96BZ4
A	36	LYS	-	expression tag	UNP Q96BZ4
A	37	LEU	-	expression tag	UNP Q96BZ4
A	38	ILE	-	expression tag	UNP Q96BZ4
A	39	SER	-	expression tag	UNP Q96BZ4
A	40	GLU	-	expression tag	UNP Q96BZ4
A	41	GLU	-	expression tag	UNP Q96BZ4
A	42	ASP	-	expression tag	UNP Q96BZ4
A	43	LEU	-	expression tag	UNP Q96BZ4
A	44	ALA	-	expression tag	UNP Q96BZ4
A	45	SER	-	expression tag	UNP Q96BZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	46	MET	-	expression tag	UNP Q96BZ4
A	47	THR	-	expression tag	UNP Q96BZ4
A	48	GLY	-	expression tag	UNP Q96BZ4
A	49	GLY	-	expression tag	UNP Q96BZ4
A	50	GLN	-	expression tag	UNP Q96BZ4
A	51	GLN	-	expression tag	UNP Q96BZ4
A	52	MET	-	expression tag	UNP Q96BZ4
A	53	GLY	-	expression tag	UNP Q96BZ4
A	54	ARG	-	expression tag	UNP Q96BZ4
A	55	ASP	-	expression tag	UNP Q96BZ4
A	56	ILE	-	expression tag	UNP Q96BZ4
A	57	GLU	-	expression tag	UNP Q96BZ4
A	58	GLY	-	expression tag	UNP Q96BZ4
A	59	ARG	-	expression tag	UNP Q96BZ4

- Molecule 2 is a protein called 5'-3' exonuclease PLD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	392	Total	C	N	O	S	0	0	0
			3053	1947	535	559	12			

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	19	HIS	-	expression tag	UNP Q96BZ4
B	20	HIS	-	expression tag	UNP Q96BZ4
B	21	HIS	-	expression tag	UNP Q96BZ4
B	22	HIS	-	expression tag	UNP Q96BZ4
B	23	HIS	-	expression tag	UNP Q96BZ4
B	24	HIS	-	expression tag	UNP Q96BZ4
B	25	GLY	-	expression tag	UNP Q96BZ4
B	26	PRO	-	expression tag	UNP Q96BZ4
B	27	LEU	-	expression tag	UNP Q96BZ4
B	28	VAL	-	expression tag	UNP Q96BZ4
B	29	ASP	-	expression tag	UNP Q96BZ4
B	30	VAL	-	expression tag	UNP Q96BZ4
B	31	ALA	-	expression tag	UNP Q96BZ4
B	32	SER	-	expression tag	UNP Q96BZ4
B	33	ASN	-	expression tag	UNP Q96BZ4
B	34	GLU	-	expression tag	UNP Q96BZ4
B	35	GLN	-	expression tag	UNP Q96BZ4
B	36	LYS	-	expression tag	UNP Q96BZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	37	LEU	-	expression tag	UNP Q96BZ4
B	38	ILE	-	expression tag	UNP Q96BZ4
B	39	SER	-	expression tag	UNP Q96BZ4
B	40	GLU	-	expression tag	UNP Q96BZ4
B	41	GLU	-	expression tag	UNP Q96BZ4
B	42	ASP	-	expression tag	UNP Q96BZ4
B	43	LEU	-	expression tag	UNP Q96BZ4
B	44	ALA	-	expression tag	UNP Q96BZ4
B	45	SER	-	expression tag	UNP Q96BZ4
B	46	MET	-	expression tag	UNP Q96BZ4
B	47	THR	-	expression tag	UNP Q96BZ4
B	48	GLY	-	expression tag	UNP Q96BZ4
B	49	GLY	-	expression tag	UNP Q96BZ4
B	50	GLN	-	expression tag	UNP Q96BZ4
B	51	GLN	-	expression tag	UNP Q96BZ4
B	52	MET	-	expression tag	UNP Q96BZ4
B	53	GLY	-	expression tag	UNP Q96BZ4
B	54	ARG	-	expression tag	UNP Q96BZ4
B	55	ASP	-	expression tag	UNP Q96BZ4
B	56	ILE	-	expression tag	UNP Q96BZ4
B	57	GLU	-	expression tag	UNP Q96BZ4
B	58	GLY	-	expression tag	UNP Q96BZ4
B	59	ARG	-	expression tag	UNP Q96BZ4

- Molecule 3 is a DNA chain called ssDNA.

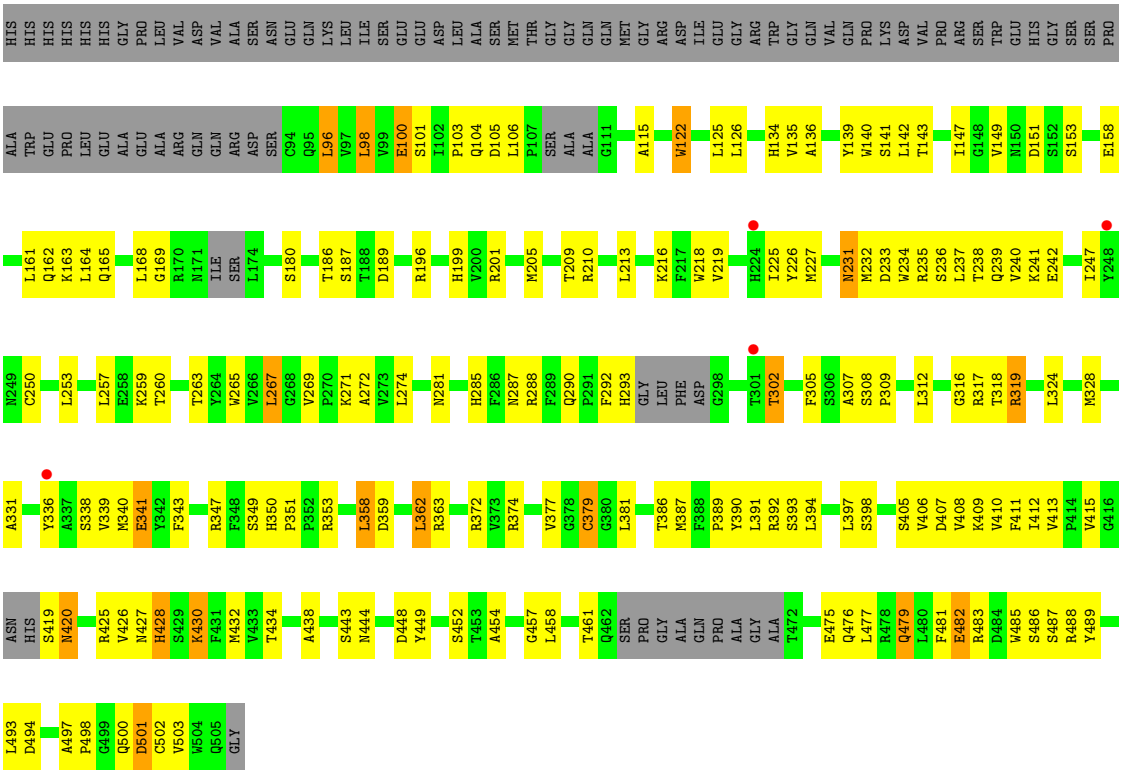
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	P	0	0	0
			57	30	6	19	2			
3	D	3	Total	C	N	O	P	0	0	0
			57	30	6	19	2			

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.

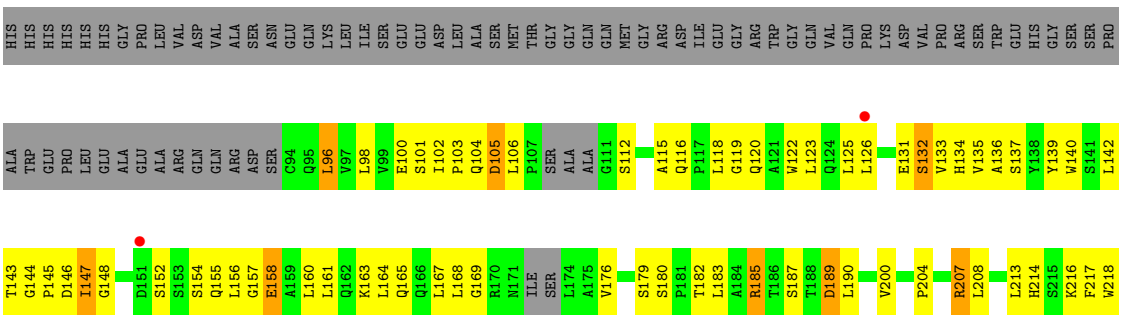
• Molecule 1: 5'-3' exonuclease PLD4

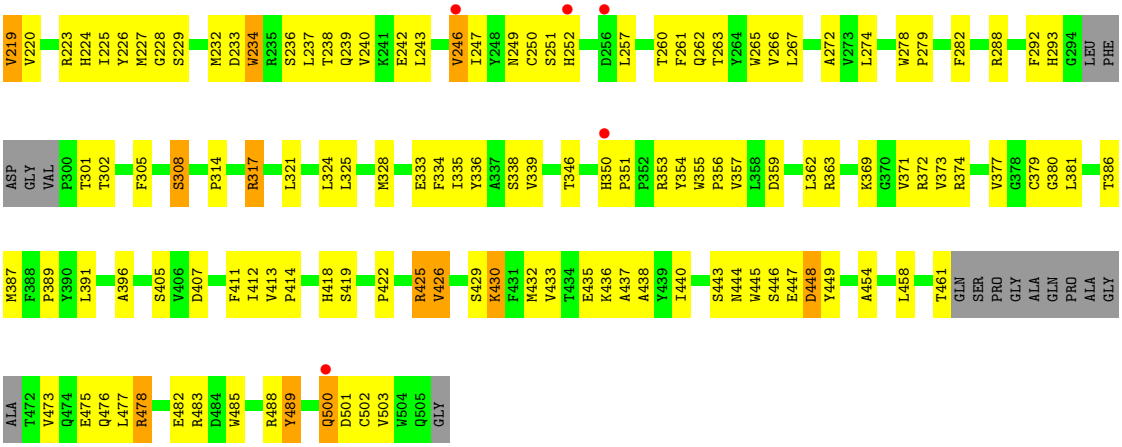
Chain A:



• Molecule 2: 5'-3' exonuclease PLD4

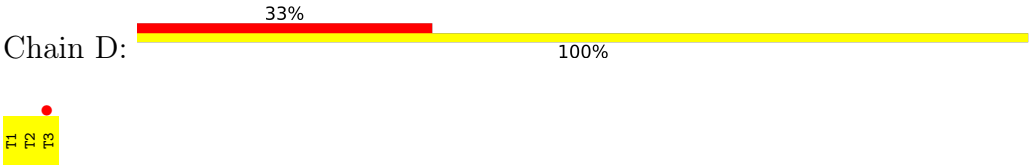
Chain B:





• Molecule 3: ssDNA

• Molecule 3: ssDNA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	88.98Å 88.98Å 273.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.66 – 3.00 44.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.66-3.00) 99.8 (44.66-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.263 , 0.318 0.269 , 0.322	Depositor DCC
R_{free} test set	1299 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	110.2	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 80.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6232	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NEP

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	0.30	0/3130	0.62	0/4263
2	B	0.32	0/3133	0.62	1/4269 (0.0%)
3	C	0.48	0/62	1.33	0/94
3	D	0.70	0/62	1.47	1/94 (1.1%)
All	All	0.32	0/6387	0.64	2/8720 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	425	ARG	CA-CB-CG	-8.21	95.34	113.40
3	D	3	DT	O4'-C1'-N1	6.11	112.28	108.00

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	3065	0	3009	126	0
2	B	3053	0	2988	144	0
3	C	57	0	38	1	0
3	D	57	0	38	2	0
All	All	6232	0	6073	270	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 22.

All (270) 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)
2:B:158:GLU:HA	2:B:161:LEU:HD13	1.47	0.96
2:B:161:LEU:HA	2:B:164:LEU:HD23	1.53	0.87
1:A:201:ARG:NH1	1:A:265:TRP:O	2.13	0.81
1:A:140:TRP:HE3	1:A:142:LEU:HD11	1.46	0.78
2:B:133:VAL:HG22	2:B:220:VAL:HG13	1.69	0.75
1:A:106:LEU:HB2	1:A:488:ARG:HH22	1.50	0.75
2:B:380:GLY:HA3	2:B:426:VAL:HG13	1.69	0.75
2:B:142:LEU:HA	2:B:234:TRP:HD1	1.53	0.74
2:B:336:TYR:O	2:B:432:MET:HA	1.87	0.73
2:B:180:SER:HB3	2:B:213:LEU:HB3	1.71	0.73
2:B:333:GLU:N	2:B:435:GLU:OE1	2.21	0.73
2:B:433:VAL:HG11	2:B:477:LEU:HB3	1.73	0.71
1:A:393:SER:OG	2:B:363:ARG:NH2	2.24	0.71
2:B:236:SER:HA	2:B:240:VAL:HG12	1.70	0.71
1:A:140:TRP:CE3	1:A:142:LEU:HD11	2.26	0.70
1:A:324:LEU:O	1:A:328:MET:HG3	1.92	0.69
2:B:112:SER:HB3	2:B:483:ARG:HG3	1.73	0.69
2:B:134:HIS:HB2	2:B:219:VAL:HG13	1.73	0.69
1:A:408:VAL:HB	1:A:493:LEU:HD11	1.76	0.68
2:B:96:LEU:HB2	2:B:247:ILE:HG12	1.76	0.68
3:C:1:DT:H2"	3:C:2:DT:H5"	1.77	0.67
2:B:100:GLU:HB2	2:B:115:ALA:HB3	1.75	0.67
2:B:448:ASP:OD1	2:B:448:ASP:N	2.30	0.65
2:B:208:LEU:HB3	2:B:274:LEU:HD21	1.79	0.65
2:B:157:GLY:HA3	2:B:234:TRP:HB3	1.79	0.64
2:B:102:ILE:HD12	2:B:106:LEU:HD22	1.79	0.64
1:A:377:VAL:HG21	1:A:391:LEU:HD21	1.80	0.63
1:A:328:MET:HE1	1:A:362:LEU:HD22	1.81	0.63
1:A:398:SER:OG	1:A:406:VAL:O	2.16	0.62
1:A:106:LEU:HB2	1:A:488:ARG:NH2	2.13	0.62
1:A:201:ARG:HG3	1:A:265:TRP:CZ3	2.35	0.62
1:A:381:LEU:HD21	1:A:501:ASP:HB2	1.80	0.62
2:B:135:VAL:HG22	2:B:218:TRP:CD1	2.35	0.62
2:B:502:CYS:SG	2:B:503:VAL:N	2.73	0.62
1:A:139:TYR:O	1:A:232:MET:HB2	1.99	0.62
1:A:236:SER:HA	1:A:240:VAL:HG12	1.82	0.61
1:A:359:ASP:O	1:A:363:ARG:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:THR:O	2:B:185:ARG:NH1	2.34	0.61
1:A:100:GLU:HB3	1:A:115:ALA:HB3	1.81	0.60
2:B:233:ASP:O	2:B:236:SER:OG	2.15	0.60
1:A:336:TYR:O	1:A:432:MET:HA	2.01	0.59
2:B:227:MET:HE1	2:B:440:ILE:O	2.02	0.59
2:B:335:ILE:HG13	2:B:371:VAL:HG11	1.83	0.59
1:A:180:SER:HB2	1:A:213:LEU:H	1.67	0.59
2:B:249:ASN:O	2:B:251:SER:N	2.35	0.59
1:A:374:ARG:HB3	1:A:485:TRP:CZ3	2.38	0.59
1:A:415:VAL:HA	1:A:425:ARG:HD2	1.84	0.59
1:A:218:TRP:HE1	1:A:232:MET:HE1	1.68	0.59
2:B:142:LEU:HB3	2:B:161:LEU:HD11	1.85	0.58
1:A:161:LEU:HA	1:A:164:LEU:HD23	1.84	0.58
1:A:227:MET:HE1	1:A:457:GLY:HA2	1.84	0.58
1:A:227:MET:HE2	1:A:458:LEU:H	1.67	0.58
1:A:419:SER:OG	1:A:420:ASN:N	2.36	0.58
2:B:279:PRO:HD2	2:B:282:PHE:CD2	2.38	0.58
1:A:377:VAL:HG23	1:A:410:VAL:HG23	1.86	0.58
2:B:263:THR:O	2:B:267:LEU:HD12	2.04	0.58
2:B:338:SER:O	2:B:430:LYS:HA	2.04	0.57
2:B:176:VAL:HG12	2:B:261:PHE:HZ	1.69	0.57
1:A:263:THR:O	1:A:267:LEU:HD12	2.04	0.57
2:B:189:ASP:OD1	2:B:189:ASP:N	2.36	0.57
2:B:225:ILE:HB	2:B:257:LEU:HD21	1.87	0.57
2:B:104:GLN:HG2	2:B:105:ASP:OD1	2.05	0.56
2:B:136:ALA:O	2:B:216:LYS:HA	2.05	0.56
1:A:260:THR:O	1:A:263:THR:OG1	2.21	0.56
2:B:411:PHE:CE1	2:B:489:TYR:HB2	2.41	0.56
1:A:341:GLU:HA	1:A:387:MET:HE1	1.88	0.55
2:B:155:GLN:HA	2:B:158:GLU:OE1	2.06	0.55
1:A:339:VAL:HG12	1:A:430:LYS:HB3	1.87	0.55
2:B:156:LEU:HD12	2:B:156:LEU:H	1.71	0.55
2:B:139:TYR:O	2:B:232:MET:HB2	2.07	0.55
1:A:101:SER:HB3	1:A:242:GLU:HB2	1.89	0.55
2:B:262:GLN:O	2:B:266:VAL:HG23	2.07	0.55
2:B:362:LEU:HD12	2:B:373:VAL:HG21	1.88	0.55
1:A:481:PHE:CE1	1:A:485:TRP:HB2	2.43	0.54
2:B:339:VAL:HG11	2:B:445:TRP:CD1	2.42	0.54
2:B:260:THR:O	2:B:263:THR:N	2.41	0.54
2:B:359:ASP:OD1	2:B:363:ARG:NH1	2.40	0.54
2:B:122:TRP:HB3	2:B:160:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:ILE:HD12	2:B:500:GLN:HG2	1.90	0.54
2:B:103:PRO:HG3	2:B:240:VAL:N	2.23	0.54
2:B:118:LEU:HD23	2:B:237:LEU:HD23	1.90	0.54
1:A:415:VAL:HB	1:A:419:SER:HB2	1.89	0.54
1:A:143:THR:HA	1:A:158:GLU:HG3	1.90	0.53
2:B:116:GLN:HE22	2:B:120:GLN:HB3	1.72	0.53
1:A:287:ASN:HB2	1:A:318:THR:HG23	1.89	0.53
1:A:305:PHE:HE1	1:A:458:LEU:HB2	1.73	0.53
1:A:392:ARG:HB3	2:B:396:ALA:HB1	1.90	0.53
2:B:336:TYR:HE2	2:B:478:ARG:HD2	1.72	0.53
1:A:134:HIS:HB2	1:A:219:VAL:HG13	1.91	0.53
2:B:374:ARG:HB3	2:B:485:TRP:CH2	2.43	0.53
3:D:1:DT:H2"	3:D:2:DT:H5"	1.90	0.53
1:A:103:PRO:HB3	1:A:239:GLN:HA	1.89	0.53
1:A:210:ARG:HH22	1:A:353:ARG:HH22	1.54	0.53
2:B:101:SER:HB2	2:B:242:GLU:HB2	1.91	0.53
1:A:350:HIS:HB2	1:A:351:PRO:HD3	1.91	0.53
2:B:260:THR:O	2:B:261:PHE:C	2.48	0.53
1:A:225:ILE:HG13	1:A:247:ILE:HB	1.91	0.53
2:B:374:ARG:HA	2:B:407:ASP:O	2.09	0.52
1:A:338:SER:O	1:A:430:LYS:HA	2.10	0.52
1:A:180:SER:HB3	1:A:213:LEU:HB3	1.90	0.52
2:B:372:ARG:HA	2:B:405:SER:HB3	1.92	0.52
1:A:216:LYS:HG2	1:A:231:ASN:HB3	1.90	0.52
1:A:448:ASP:N	1:A:448:ASP:OD1	2.41	0.52
1:A:502:CYS:SG	1:A:503:VAL:N	2.82	0.52
1:A:257:LEU:HD22	1:A:305:PHE:CE2	2.44	0.52
2:B:143:THR:O	2:B:145:PRO:HD2	2.09	0.52
2:B:346:THR:HG22	2:B:353:ARG:H	1.75	0.51
2:B:292:PHE:O	2:B:302:THR:OG1	2.21	0.51
1:A:339:VAL:O	1:A:377:VAL:HA	2.11	0.51
2:B:239:GLN:OE1	2:B:425:ARG:NH2	2.32	0.51
2:B:350:HIS:HB2	2:B:351:PRO:HD3	1.93	0.51
1:A:438:ALA:HB1	1:A:477:LEU:HD12	1.92	0.51
1:A:287:ASN:HB3	1:A:316:GLY:O	2.11	0.51
2:B:437:ALA:HA	2:B:461:THR:HG22	1.92	0.51
1:A:227:MET:CE	1:A:457:GLY:HA2	2.40	0.51
1:A:374:ARG:HB3	1:A:485:TRP:CH2	2.46	0.51
2:B:207:ARG:NH2	2:B:272:ALA:O	2.42	0.50
1:A:305:PHE:CE1	1:A:458:LEU:HB2	2.45	0.50
1:A:340:MET:SD	1:A:428:NEP:HD2	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:SER:OG	2:B:189:ASP:OD1	2.28	0.50
2:B:219:VAL:HB	2:B:257:LEU:HD11	1.92	0.50
1:A:122:TRP:O	1:A:126:LEU:HD22	2.12	0.50
1:A:151:ASP:OD1	1:A:153:SER:OG	2.28	0.50
2:B:239:GLN:HA	2:B:425:ARG:HH12	1.76	0.50
1:A:153:SER:O	1:A:238:THR:HG21	2.12	0.49
2:B:131:GLU:HG3	2:B:132:SER:HB3	1.94	0.49
2:B:501:ASP:N	2:B:501:ASP:OD1	2.45	0.49
1:A:253:LEU:HD21	1:A:292:PHE:HB2	1.94	0.49
1:A:125:LEU:HD23	1:A:218:TRP:HE3	1.77	0.49
2:B:354:TYR:CE2	2:B:356:PRO:HB3	2.48	0.49
2:B:475:GLU:HA	2:B:478:ARG:HB2	1.93	0.49
2:B:377:VAL:HG21	2:B:391:LEU:HD11	1.95	0.49
1:A:103:PRO:HD2	1:A:105:ASP:OD2	2.12	0.49
1:A:309:PRO:HD2	1:A:312:LEU:HG	1.94	0.49
1:A:372:ARG:HA	1:A:405:SER:HB3	1.95	0.49
1:A:227:MET:HE1	1:A:457:GLY:CA	2.42	0.49
2:B:125:LEU:HD12	2:B:220:VAL:HG21	1.95	0.48
2:B:239:GLN:CA	2:B:425:ARG:HH12	2.26	0.48
2:B:137:SER:OG	2:B:140:TRP:NE1	2.45	0.48
1:A:210:ARG:HD2	1:A:452:SER:HB2	1.96	0.48
1:A:302:THR:HG23	1:A:461:THR:HG23	1.95	0.48
1:A:307:ALA:O	1:A:319:ARG:HA	2.13	0.48
1:A:103:PRO:O	1:A:105:ASP:N	2.46	0.48
1:A:213:LEU:HA	1:A:454:ALA:HB3	1.96	0.48
2:B:156:LEU:HD13	2:B:238:THR:HB	1.96	0.48
1:A:139:TYR:HE1	1:A:233:ASP:HB2	1.79	0.48
2:B:176:VAL:HG13	2:B:265:TRP:CH2	2.49	0.48
1:A:483:ARG:O	1:A:487:SER:HB2	2.13	0.47
2:B:377:VAL:HG21	2:B:391:LEU:CD1	2.43	0.47
2:B:180:SER:O	2:B:182:THR:OG1	2.28	0.47
2:B:226:TYR:HB2	2:B:246:VAL:HG13	1.97	0.47
1:A:236:SER:HA	1:A:240:VAL:CG1	2.44	0.47
1:A:141:SER:O	1:A:233:ASP:HA	2.15	0.47
2:B:223:ARG:HD3	2:B:251:SER:HB3	1.97	0.47
2:B:473:VAL:HA	2:B:476:GLN:HG3	1.96	0.47
1:A:98:LEU:HD11	1:A:476:GLN:NE2	2.30	0.47
1:A:487:SER:OG	1:A:488:ARG:N	2.46	0.47
2:B:157:GLY:O	2:B:160:LEU:HB3	2.14	0.47
2:B:217:PHE:HE1	2:B:261:PHE:HB2	1.79	0.47
2:B:279:PRO:HD2	2:B:282:PHE:HD2	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:VAL:HG12	2:B:438:ALA:HA	1.97	0.46
1:A:142:LEU:HD12	1:A:189:ASP:OD2	2.15	0.46
2:B:308:SER:O	2:B:454:ALA:HA	2.15	0.46
2:B:336:TYR:HE2	2:B:478:ARG:CD	2.28	0.46
2:B:435:GLU:HG2	2:B:436:LYS:HD2	1.97	0.46
2:B:204:PRO:O	2:B:207:ARG:HB2	2.15	0.46
1:A:165:GLN:HA	1:A:196:ARG:NH2	2.30	0.46
1:A:475:GLU:OE2	1:A:479:GLN:NE2	2.48	0.46
2:B:216:LYS:HG3	2:B:228:GLY:O	2.16	0.46
2:B:225:ILE:HD12	2:B:225:ILE:O	2.16	0.46
1:A:205:MET:CE	1:A:454:ALA:HB2	2.46	0.46
2:B:243:LEU:HB3	2:B:429:SER:HB2	1.98	0.46
1:A:136:ALA:O	1:A:216:LYS:HA	2.16	0.46
1:A:269:VAL:HG12	1:A:272:ALA:HB2	1.98	0.46
2:B:164:LEU:O	2:B:168:LEU:HD12	2.16	0.46
2:B:336:TYR:OH	2:B:374:ARG:NH1	2.48	0.46
2:B:144:GLY:HA2	2:B:234:TRP:CZ2	2.51	0.46
1:A:443:SER:HB3	1:A:449:TYR:HB3	1.97	0.46
1:A:96:LEU:HB2	1:A:247:ILE:HG12	1.97	0.45
1:A:500:GLN:OE1	1:A:500:GLN:N	2.33	0.45
2:B:142:LEU:HA	2:B:234:TRP:CD1	2.42	0.45
1:A:343:PHE:CD2	1:A:347[A]:ARG:HD2	2.51	0.45
1:A:497:ALA:N	1:A:500:GLN:HE22	2.13	0.45
2:B:334:PHE:HB2	2:B:336:TYR:CE1	2.50	0.45
1:A:259:LYS:NZ	1:A:281:ASN:O	2.46	0.45
1:A:407:ASP:HB3	1:A:485:TRP:CZ2	2.51	0.45
2:B:257:LEU:HD23	2:B:305:PHE:CZ	2.52	0.45
1:A:379:CYS:HB2	1:A:410:VAL:HG22	1.98	0.45
1:A:274:LEU:HD21	1:A:312:LEU:HD23	1.99	0.45
1:A:135:VAL:HG22	1:A:218:TRP:CD1	2.51	0.45
1:A:444:ASN:HB2	1:A:449:TYR:CE2	2.51	0.45
2:B:444:ASN:HB2	2:B:449:TYR:CE2	2.52	0.45
1:A:394:LEU:O	1:A:397:LEU:HB2	2.17	0.45
2:B:190:LEU:HD13	2:B:200:VAL:HG11	1.99	0.45
2:B:119:GLY:O	2:B:123:LEU:HG	2.17	0.44
2:B:229:SER:OG	2:B:242:GLU:OE2	2.23	0.44
1:A:140:TRP:CD2	1:A:232:MET:HG3	2.52	0.44
1:A:162:GLN:OE1	1:A:162:GLN:HA	2.16	0.44
2:B:143:THR:HG22	2:B:161:LEU:HD21	1.98	0.44
2:B:346:THR:CG2	2:B:353:ARG:H	2.30	0.44
2:B:125:LEU:HD21	2:B:246:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:LEU:HA	2:B:454:ALA:HB3	1.99	0.44
2:B:354:TYR:HE2	2:B:356:PRO:HB3	1.82	0.44
1:A:292:PHE:O	1:A:293:HIS:HD2	2.00	0.44
2:B:278:TRP:HB2	2:B:314:PRO:HB3	2.00	0.44
1:A:233:ASP:OD2	1:A:235:ARG:HB2	2.18	0.44
1:A:168:LEU:HB2	1:A:196:ARG:HH22	1.82	0.44
1:A:331:ALA:HB2	1:A:434:THR:HG21	2.00	0.44
2:B:183:LEU:HD13	3:D:1:DT:C2	2.53	0.44
2:B:324:LEU:O	2:B:328:MET:HG3	2.18	0.44
2:B:158:GLU:O	2:B:161:LEU:HB2	2.18	0.43
1:A:180:SER:CB	1:A:213:LEU:H	2.32	0.43
2:B:336:TYR:CZ	2:B:374:ARG:NH1	2.76	0.43
2:B:386:THR:O	2:B:389:PRO:HD2	2.19	0.43
1:A:489:TYR:N	1:A:489:TYR:CD1	2.86	0.43
2:B:143:THR:C	2:B:145:PRO:HD2	2.39	0.43
1:A:374:ARG:HA	1:A:407:ASP:O	2.18	0.43
1:A:386:THR:O	1:A:389:PRO:HD2	2.18	0.43
1:A:363:ARG:NH1	1:A:397:LEU:HD21	2.34	0.43
2:B:414:PRO:HA	2:B:501:ASP:OD2	2.19	0.43
1:A:147:ILE:HD11	1:A:234:TRP:HZ2	1.84	0.43
2:B:477:LEU:HD23	2:B:477:LEU:O	2.19	0.42
1:A:209:THR:O	1:A:209:THR:OG1	2.31	0.42
1:A:426:VAL:HG22	1:A:427:ASN:N	2.33	0.42
2:B:305:PHE:C	2:B:317:ARG:HH22	2.23	0.42
1:A:140:TRP:CE3	1:A:232:MET:HG3	2.54	0.42
1:A:290:GLN:HG2	1:A:290:GLN:O	2.20	0.42
1:A:413:VAL:HG23	1:A:425:ARG:HD3	2.00	0.42
2:B:321:LEU:O	2:B:325:LEU:HG	2.20	0.42
1:A:482:GLU:OE1	1:A:486:SER:OG	2.36	0.42
2:B:257:LEU:O	2:B:260:THR:OG1	2.34	0.42
1:A:165:GLN:O	1:A:169:GLY:N	2.47	0.42
2:B:218:TRP:HB2	2:B:226:TYR:HB3	2.02	0.42
2:B:305:PHE:CZ	2:B:458:LEU:HD22	2.54	0.42
1:A:412:ILE:HD12	1:A:500:GLN:HG3	2.02	0.42
2:B:104:GLN:OE1	2:B:418:HIS:NE2	2.53	0.42
2:B:147:ILE:HG13	2:B:148:GLY:O	2.19	0.42
2:B:227:MET:HE1	2:B:458:LEU:H	1.85	0.42
1:A:239:GLN:HA	1:A:239:GLN:OE1	2.20	0.42
2:B:135:VAL:HG22	2:B:218:TRP:NE1	2.34	0.42
2:B:142:LEU:CA	2:B:234:TRP:HD1	2.28	0.42
2:B:355:TRP:CD1	2:B:447:GLU:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:VAL:HA	2:B:414:PRO:HD3	1.91	0.42
2:B:339:VAL:HG11	2:B:445:TRP:NE1	2.35	0.41
1:A:359:ASP:OD1	1:A:363:ARG:NE	2.51	0.41
2:B:118:LEU:HD21	2:B:122:TRP:CZ2	2.55	0.41
2:B:328:MET:HG2	2:B:432:MET:SD	2.60	0.41
1:A:140:TRP:CE2	1:A:232:MET:HG3	2.56	0.41
1:A:497:ALA:HA	1:A:498:PRO:HD2	1.93	0.41
2:B:380:GLY:O	2:B:381:LEU:HB2	2.21	0.41
2:B:443:SER:HB3	2:B:449:TYR:HB3	2.02	0.41
1:A:409:LYS:HG3	1:A:485:TRP:CH2	2.55	0.41
2:B:223:ARG:O	2:B:223:ARG:HG3	2.20	0.41
1:A:488:ARG:NH2	1:A:489:TYR:OH	2.53	0.41
1:A:241:LYS:HB3	1:A:427:ASN:HA	2.01	0.41
1:A:411:PHE:CE1	1:A:489:TYR:HB2	2.55	0.41
2:B:239:GLN:O	2:B:425:ARG:NH1	2.54	0.41
2:B:369:LYS:HB3	2:B:369:LYS:HE3	1.72	0.41
2:B:134:HIS:ND1	2:B:176:VAL:HB	2.35	0.41
2:B:214:HIS:O	2:B:216:LYS:HE3	2.21	0.41
2:B:279:PRO:HD2	2:B:282:PHE:CE2	2.56	0.41
2:B:288:ARG:HE	2:B:288:ARG:HB3	1.66	0.41
2:B:165:GLN:O	2:B:169:GLY:N	2.50	0.41
2:B:334:PHE:HA	2:B:372:ARG:O	2.21	0.41
1:A:358:LEU:HA	1:A:358:LEU:HD13	1.78	0.40
1:A:237:LEU:HD23	1:A:237:LEU:HA	1.87	0.40
2:B:122:TRP:CD2	2:B:218:TRP:HH2	2.39	0.40
2:B:301:THR:HA	2:B:461:THR:O	2.21	0.40
1:A:390:TYR:O	1:A:393:SER:HB3	2.21	0.40
1:A:147:ILE:HG13	1:A:149:VAL:HG13	2.04	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	380/488 (78%)	352 (93%)	27 (7%)	1 (0%)	41 76
2	B	382/488 (78%)	350 (92%)	29 (8%)	3 (1%)	19 57
All	All	762/976 (78%)	702 (92%)	56 (7%)	4 (0%)	29 68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	250	CYS
1	A	104	GLN
2	B	105	ASP
2	B	422	PRO

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	331/405 (82%)	301 (91%)	30 (9%)	9 34
2	B	331/406 (82%)	295 (89%)	36 (11%)	6 25
All	All	662/811 (82%)	596 (90%)	66 (10%)	7 29

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	98	LEU
1	A	100	GLU
1	A	122	TRP
1	A	163	LYS
1	A	186	THR
1	A	187	SER
1	A	199	HIS
1	A	226	TYR
1	A	231	ASN
1	A	250	CYS
1	A	267	LEU

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Mol	Chain	Res	Type
1	A	271	LYS
1	A	285	HIS
1	A	288	ARG
1	A	302	THR
1	A	308	SER
1	A	317	ARG
1	A	319	ARG
1	A	341	GLU
1	A	349	SER
1	A	358	LEU
1	A	362	LEU
1	A	379	CYS
1	A	420	ASN
1	A	430	LYS
1	A	479	GLN
1	A	482	GLU
1	A	494	ASP
1	A	501	ASP
2	B	96	LEU
2	B	98	LEU
2	B	126	LEU
2	B	132	SER
2	B	146	ASP
2	B	147	ILE
2	B	152	SER
2	B	154	SER
2	B	158	GLU
2	B	163	LYS
2	B	167	LEU
2	B	179	SER
2	B	185	ARG
2	B	189	ASP
2	B	207	ARG
2	B	219	VAL
2	B	224	HIS
2	B	234	TRP
2	B	246	VAL
2	B	252	HIS
2	B	293	HIS
2	B	308	SER
2	B	317	ARG
2	B	357	VAL

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Mol	Chain	Res	Type
2	B	379	CYS
2	B	387	MET
2	B	419	SER
2	B	426	VAL
2	B	430	LYS
2	B	446	SER
2	B	448	ASP
2	B	478	ARG
2	B	482	GLU
2	B	488	ARG
2	B	489	TYR
2	B	500	GLN

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

Mol	Chain	Res	Type
1	A	293	HIS
1	A	476	GLN
2	B	116	GLN
2	B	231	ASN
2	B	249	ASN
2	B	428	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\|>2$
1	NEP	A	428	1	10,14,15	5.35	4 (40%)	5,20,22	3.81	2 (40%)

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
1	NEP	A	428	1	-	2/5/12/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	428	NEP	P-O3P	15.61	1.60	1.47
1	A	428	NEP	P-O2P	-4.37	1.45	1.54
1	A	428	NEP	P-O1P	3.12	1.61	1.54
1	A	428	NEP	CD2-CG	2.93	1.40	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	428	NEP	O1P-P-O3P	-8.10	95.92	113.44
1	A	428	NEP	CB-CA-C	-2.27	107.22	111.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	428	NEP	CA-CB-CG-ND1
1	A	428	NEP	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	428	NEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	391/488 (80%)	-0.09	4 (1%) 82 59	68, 117, 161, 202	0
2	B	392/488 (80%)	-0.05	7 (1%) 68 40	30, 130, 175, 236	0
3	C	3/3 (100%)	1.01	0 100 100	130, 130, 133, 161	0
3	D	3/3 (100%)	1.62	1 (33%) 0 0	174, 174, 188, 204	0
All	All	789/982 (80%)	-0.06	12 (1%) 73 46	30, 122, 171, 236	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	126	LEU	3.5
1	A	248	TYR	3.0
3	D	3	DT	2.9
2	B	256	ASP	2.3
1	A	301	THR	2.3
2	B	246	VAL	2.3
2	B	151	ASP	2.2
2	B	252	HIS	2.2
2	B	350	HIS	2.2
2	B	500	GLN	2.2
1	A	224	HIS	2.1
1	A	336	TYR	2.1

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, 95^{th} 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
1	NEP	A	428	14/15	0.92	0.17	85,102,144,173	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.