



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:02 PM GMT

PDB ID : 3QQS
Title : Anthranilate phosphoribosyltransferase (TRPD) from Mycobacterium tuberculosis (complex with inhibitor ACS172)
Authors : Castell, A.; Short, F.L.; Lott, J.S.; TB Structural Genomics Consortium (TB-SGC)
Deposited on : 2011-02-16
Resolution : 1.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

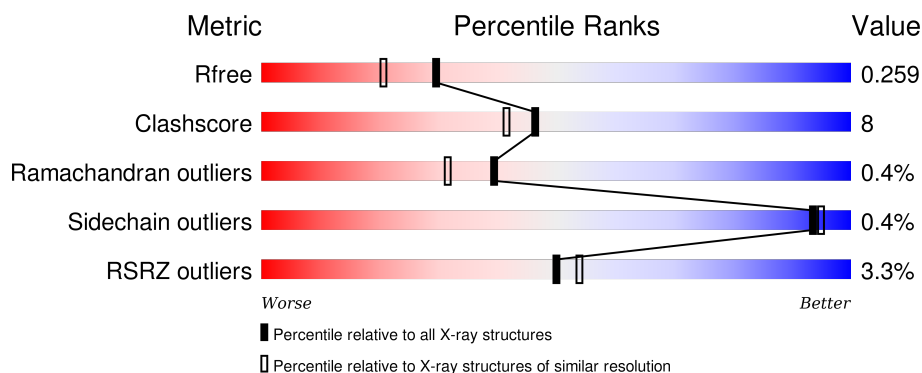
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	377	<div> <div>2%</div> <div>83% 8% 8%</div> </div>
1	B	377	<div> <div>%</div> <div>82% 9% 8%</div> </div>
1	C	377	<div> <div>5%</div> <div>73% 17% 9%</div> </div>
1	D	377	<div> <div>4%</div> <div>74% 13% 12%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	17C	C	404	-	-	-	X
4	17C	D	403	-	-	-	X
5	DPO	D	401	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10712 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 Anthranilate phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2505	1566	465	465	9			
1	B	346	Total	C	N	O	S	0	0	0
			2505	1566	465	465	9			
1	C	343	Total	C	N	O	S	0	0	0
			2482	1552	461	460	9			
1	D	330	Total	C	N	O	S	0	0	0
			2406	1508	448	441	9			

There are 32 discrepancies between the modelled and reference sequences:

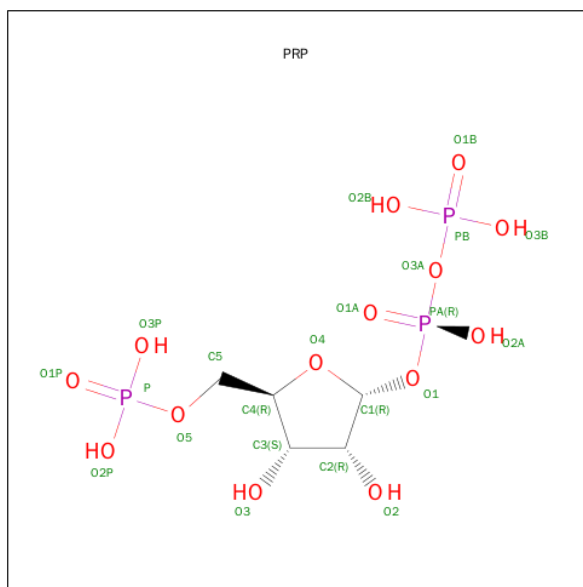
Chain	Residue	Modelled	Actual	Comment	Reference
A	371	LEU	-	EXPRESSION TAG	UNP P66992
A	372	GLU	-	EXPRESSION TAG	UNP P66992
A	373	HIS	-	EXPRESSION TAG	UNP P66992
A	374	HIS	-	EXPRESSION TAG	UNP P66992
A	375	HIS	-	EXPRESSION TAG	UNP P66992
A	376	HIS	-	EXPRESSION TAG	UNP P66992
A	377	HIS	-	EXPRESSION TAG	UNP P66992
A	378	HIS	-	EXPRESSION TAG	UNP P66992
B	371	LEU	-	EXPRESSION TAG	UNP P66992
B	372	GLU	-	EXPRESSION TAG	UNP P66992
B	373	HIS	-	EXPRESSION TAG	UNP P66992
B	374	HIS	-	EXPRESSION TAG	UNP P66992
B	375	HIS	-	EXPRESSION TAG	UNP P66992
B	376	HIS	-	EXPRESSION TAG	UNP P66992
B	377	HIS	-	EXPRESSION TAG	UNP P66992
B	378	HIS	-	EXPRESSION TAG	UNP P66992
C	371	LEU	-	EXPRESSION TAG	UNP P66992
C	372	GLU	-	EXPRESSION TAG	UNP P66992
C	373	HIS	-	EXPRESSION TAG	UNP P66992
C	374	HIS	-	EXPRESSION TAG	UNP P66992
C	375	HIS	-	EXPRESSION TAG	UNP P66992

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Chain	Residue	Modelled	Actual	Comment	Reference
C	376	HIS	-	EXPRESSION TAG	UNP P66992
C	377	HIS	-	EXPRESSION TAG	UNP P66992
C	378	HIS	-	EXPRESSION TAG	UNP P66992
D	371	LEU	-	EXPRESSION TAG	UNP P66992
D	372	GLU	-	EXPRESSION TAG	UNP P66992
D	373	HIS	-	EXPRESSION TAG	UNP P66992
D	374	HIS	-	EXPRESSION TAG	UNP P66992
D	375	HIS	-	EXPRESSION TAG	UNP P66992
D	376	HIS	-	EXPRESSION TAG	UNP P66992
D	377	HIS	-	EXPRESSION TAG	UNP P66992
D	378	HIS	-	EXPRESSION TAG	UNP P66992

- Molecule 2 is ALPHA-PHOSPHORIBOSYLPYROPHOSPHORIC ACID (three-letter code: PRP) (formula: $C_5H_{13}O_{14}P_3$).

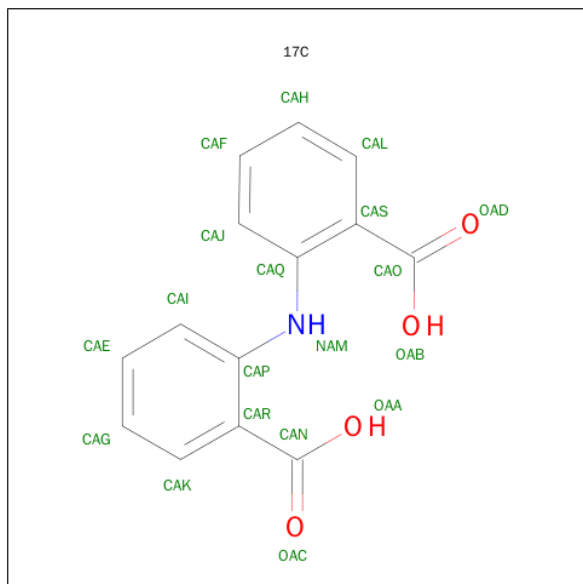


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			22	5	14	3		
2	B	1	Total	C	O	P	0	0
			22	5	14	3		
2	C	1	Total	C	O	P	0	0
			22	5	14	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

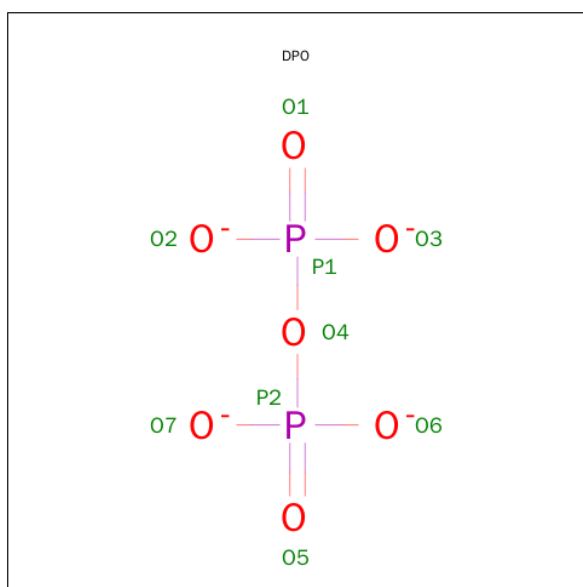
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is 2,2'-IMINODIBENZOIC ACID (three-letter code: 17C) (formula: C₁₄H₁₁NO₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 19 14 1 4	0	0
4	B	1	Total C N O 19 14 1 4	0	0
4	C	1	Total C N O 19 14 1 4	0	0
4	C	1	Total C N O 19 14 1 4	0	0
4	C	1	Total C N O 19 14 1 4	0	0
4	D	1	Total C N O 19 14 1 4	0	0
4	D	1	Total C N O 19 14 1 4	0	0

- Molecule 5 is DIPHOSPHATE (three-letter code: DPO) (formula: O₇P₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O P 9 7 2	0	0

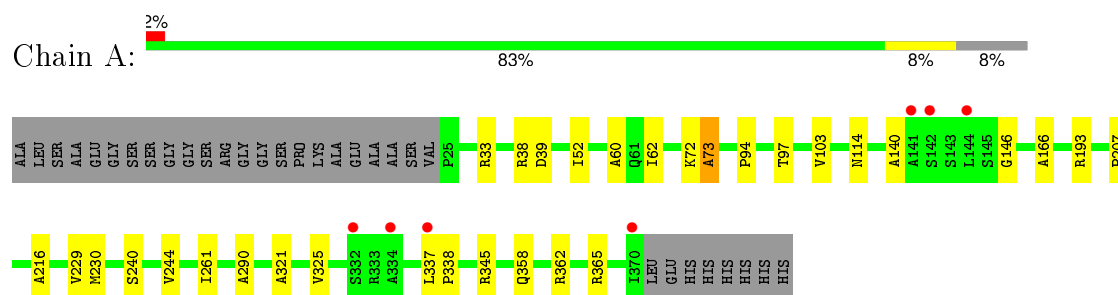
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	191	Total O 191 191	0	0
6	B	176	Total O 176 176	0	0
6	C	111	Total O 111 111	0	0
6	D	123	Total O 123 123	0	0

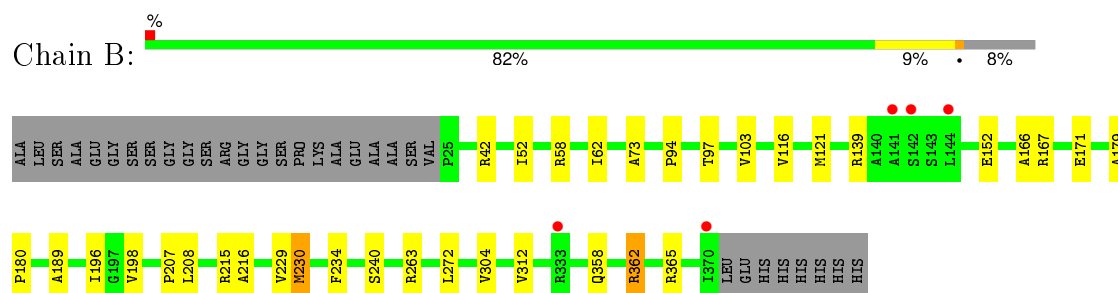
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

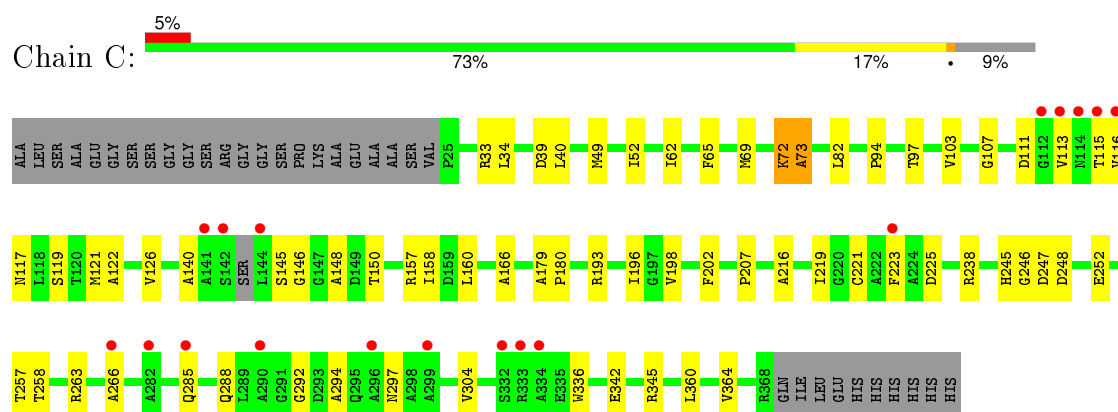
- Molecule 1: Anthranilate phosphoribosyltransferase



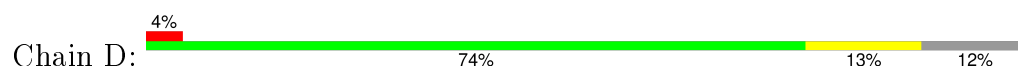
- Molecule 1: Anthranilate phosphoribosyltransferase

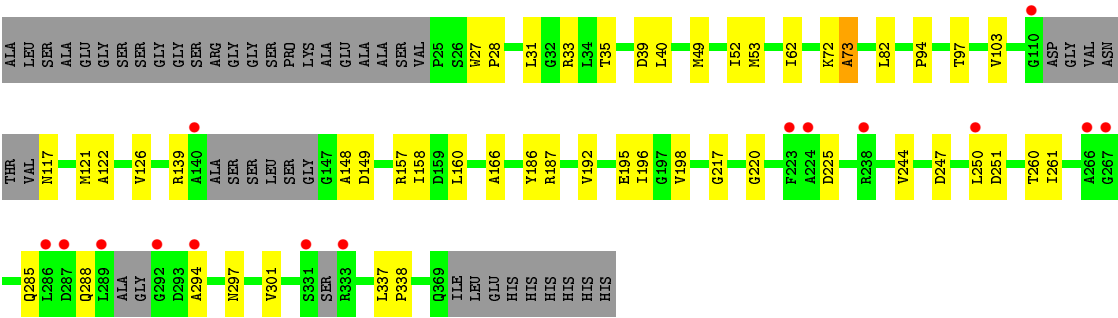


- Molecule 1: Anthranilate phosphoribosyltransferase



- Molecule 1: Anthranilate phosphoribosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.93Å 78.21Å 101.70Å 90.00° 111.01° 90.00°	Depositor
Resolution (Å)	88.75 – 1.97 60.37 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.0 (88.75-1.97) 99.0 (60.37-1.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.216 , 0.259 0.217 , 0.259	Depositor DCC
R_{free} test set	4846 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	3 of 97380 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10712	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.25 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.7047e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DPO, MG, 17C, PRP

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	0.63	0/2553	0.73	1/3483 (0.0%)
1	B	0.62	0/2553	0.72	3/3483 (0.1%)
1	C	0.52	0/2529	0.63	0/3449
1	D	0.54	0/2450	0.65	0/3336
All	All	0.58	0/10085	0.68	4/13751 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	362	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	230	MET	CG-SD-CE	-5.47	91.45	100.20
1	B	215	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	2500	20	0
1	B	2505	0	2500	24	0
1	C	2482	0	2476	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2406	0	2401	37	0
2	A	22	0	8	0	0
2	B	22	0	8	0	0
2	C	22	0	8	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
4	A	19	0	9	4	0
4	B	19	0	9	2	0
4	C	57	0	27	5	0
4	D	38	0	18	10	0
5	D	9	0	0	0	0
6	A	191	0	0	3	0
6	B	176	0	0	3	0
6	C	111	0	0	3	0
6	D	123	0	0	1	0
All	All	10712	0	9964	153	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 8.

All (153) 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:A:362:ARG:HG3	1:A:365:ARG:NH2	1.92	0.85
1:C:193:ARG:HD2	6:C:532:HOH:O	1.83	0.77
1:C:97:THR:HG23	1:C:166:ALA:HB1	1.67	0.76
1:C:117:ASN:ND2	1:C:150:THR:OG1	2.19	0.75
4:D:403:17C:HAI	4:D:403:17C:CAJ	2.19	0.72
1:B:103:VAL:HG12	1:B:216:ALA:HB3	1.71	0.72
1:A:358:GLN:O	1:A:362:ARG:HD3	1.93	0.69
1:B:229:VAL:HG23	6:B:532:HOH:O	1.91	0.69
4:D:402:17C:CAI	4:D:402:17C:HAJ	2.21	0.69
1:D:49:MET:HE2	1:D:82:LEU:HB3	1.74	0.68
1:C:34:LEU:HD11	1:C:69:MET:HE2	1.74	0.68
1:A:103:VAL:HG12	1:A:216:ALA:HB3	1.75	0.68
1:C:49:MET:CE	1:C:82:LEU:HD22	2.23	0.68
1:D:285:GLN:HB2	1:D:288:GLN:HB2	1.75	0.68
1:A:229:VAL:HG23	6:A:524:HOH:O	1.92	0.67
4:D:402:17C:CAJ	4:D:402:17C:HAI	2.24	0.66
1:C:342:GLU:HA	1:C:345:ARG:NH1	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:VAL:HA	1:C:297:ASN:ND2	2.12	0.65
4:D:402:17C:HAI	4:D:402:17C:HAJ	1.79	0.64
1:C:225:ASP:HB3	6:C:605:HOH:O	1.98	0.62
1:C:49:MET:HE3	1:C:82:LEU:HD22	1.80	0.61
1:C:97:THR:CG2	1:C:166:ALA:HB1	2.31	0.61
1:B:94:PRO:O	1:B:97:THR:HG22	2.01	0.61
1:C:238:ARG:NH2	1:C:266:ALA:O	2.33	0.61
4:D:403:17C:CAJ	4:D:403:17C:CAI	2.78	0.61
1:D:121:MET:HG2	1:D:301:VAL:HG22	1.84	0.60
1:B:116:VAL:HG22	1:B:121:MET:HE2	1.83	0.59
4:A:404:17C:HAI	4:A:404:17C:HAJ	1.84	0.59
1:B:116:VAL:HG22	1:B:121:MET:CE	2.33	0.59
1:C:148:ALA:HB1	1:C:158:ILE:HD12	1.85	0.58
4:A:404:17C:CAJ	4:A:404:17C:HAI	2.33	0.57
1:B:358:GLN:O	1:B:362:ARG:HD3	2.04	0.57
1:D:117:ASN:HB3	1:D:297:ASN:ND2	2.19	0.57
4:C:405:17C:HAI	4:C:405:17C:HAJ	1.87	0.57
1:D:94:PRO:HG2	1:D:97:THR:HG21	1.87	0.57
4:D:402:17C:CAJ	4:D:402:17C:CAI	2.77	0.57
1:B:207:PRO:HB2	1:B:230:MET:HE1	1.88	0.56
4:C:405:17C:CAJ	4:C:405:17C:HAI	2.36	0.55
1:D:97:THR:HB	1:D:166:ALA:HB1	1.87	0.55
1:D:103:VAL:HG22	1:D:217:GLY:HA2	1.87	0.55
1:C:119:SER:HB2	2:C:401:PRP:PB	2.46	0.55
1:C:196:ILE:HG23	1:C:198:VAL:HG22	1.89	0.55
1:C:246:GLY:C	1:C:248:ASP:H	2.09	0.54
1:A:52:ILE:HG12	1:A:62:ILE:HG12	1.89	0.54
1:B:42:ARG:HD3	6:B:674:HOH:O	2.08	0.54
1:C:103:VAL:HG12	1:C:216:ALA:HB3	1.89	0.53
1:D:33:ARG:HD3	1:D:39:ASP:O	2.09	0.53
1:A:337:LEU:HB2	1:A:338:PRO:HD3	1.90	0.53
1:D:196:ILE:HG22	1:D:198:VAL:HG22	1.90	0.53
1:B:216:ALA:HA	1:B:240:SER:O	2.09	0.53
1:D:157:ARG:HG2	1:D:160:LEU:HD21	1.89	0.53
1:B:196:ILE:HG22	1:B:198:VAL:HG22	1.89	0.53
4:B:404:17C:CAJ	4:B:404:17C:HAI	2.39	0.53
1:C:97:THR:CG2	1:C:166:ALA:CB	2.87	0.52
1:A:33:ARG:HD3	1:A:39:ASP:O	2.09	0.52
1:B:42:ARG:NH1	6:B:544:HOH:O	2.42	0.52
1:C:121:MET:CE	1:C:304:VAL:HB	2.39	0.52
1:C:116:VAL:HA	1:C:297:ASN:HD22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:MET:HE2	1:C:82:LEU:HD22	1.89	0.52
1:B:198:VAL:HG11	1:D:31:LEU:HB2	1.90	0.52
1:C:65:PHE:CZ	1:C:69:MET:HE3	2.45	0.51
1:D:186:TYR:CD2	4:D:403:17C:HAK	2.45	0.51
1:B:97:THR:OG1	1:B:166:ALA:HB1	2.11	0.51
1:A:33:ARG:HG2	1:A:38:ARG:HB2	1.92	0.51
1:C:65:PHE:CE1	1:C:69:MET:CE	2.94	0.51
1:B:207:PRO:HB2	1:B:230:MET:CE	2.40	0.51
1:D:103:VAL:CG2	1:D:217:GLY:HA2	2.41	0.51
1:A:140:ALA:HB2	1:A:146:GLY:N	2.26	0.51
1:D:149:ASP:OD2	1:D:294:ALA:HB2	2.10	0.50
1:C:34:LEU:CD1	1:C:69:MET:HE2	2.40	0.50
1:C:117:ASN:HB3	2:C:401:PRP:O3B	2.11	0.49
1:A:193:ARG:HG3	6:A:541:HOH:O	2.11	0.49
1:A:94:PRO:O	1:A:97:THR:HG22	2.12	0.49
1:D:121:MET:CG	1:D:301:VAL:HG22	2.42	0.49
4:B:404:17C:HAI	4:B:404:17C:HAJ	1.94	0.48
1:D:220:GLY:HA3	1:D:251:ASP:O	2.13	0.48
1:C:145:SER:OG	1:C:294:ALA:HA	2.13	0.48
1:C:221:CYS:O	1:C:245:HIS:HD2	1.95	0.48
1:C:193:ARG:HD3	1:C:202:PHE:CB	2.44	0.48
1:A:97:THR:OG1	1:A:166:ALA:HB1	2.13	0.48
1:D:49:MET:CE	1:D:82:LEU:HB3	2.42	0.48
1:B:52:ILE:HG12	1:B:62:ILE:HG12	1.96	0.48
1:A:321:ALA:O	1:A:325:VAL:HG23	2.14	0.48
1:C:119:SER:HB2	2:C:401:PRP:O3B	2.14	0.48
1:D:337:LEU:HB2	1:D:338:PRO:HD3	1.95	0.48
1:C:122:ALA:O	1:C:126:VAL:HG23	2.14	0.48
4:C:405:17C:CAI	4:C:405:17C:HAJ	2.44	0.47
1:C:113:VAL:HG12	1:C:115:THR:HG23	1.96	0.47
4:D:403:17C:HAJ	4:D:403:17C:CAI	2.44	0.47
1:B:139:ARG:NH2	1:B:152:GLU:OE1	2.47	0.47
1:A:216:ALA:HA	1:A:240:SER:O	2.14	0.47
1:B:362:ARG:HG3	1:B:365:ARG:HH21	1.80	0.47
1:D:139:ARG:HD3	1:D:149:ASP:HB3	1.96	0.47
1:C:179:ALA:HB3	1:C:180:PRO:HD3	1.96	0.47
1:B:167:ARG:O	1:B:171:GLU:HG3	2.15	0.46
1:A:114:ASN:O	1:A:290:ALA:HA	2.15	0.46
1:C:207:PRO:HB3	1:C:219:ILE:HG23	1.97	0.46
1:D:225:ASP:OD2	1:D:225:ASP:N	2.47	0.46
1:C:107:GLY:HA3	6:C:508:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:LEU:O	1:C:364:VAL:HG23	2.16	0.45
1:C:33:ARG:HD3	1:C:39:ASP:O	2.16	0.45
1:D:52:ILE:HG12	1:D:62:ILE:HG12	1.97	0.45
1:C:157:ARG:HG2	1:C:160:LEU:CD2	2.46	0.45
1:C:52:ILE:HG12	1:C:62:ILE:HG12	1.99	0.45
1:D:33:ARG:HD2	1:D:40:LEU:HD23	1.97	0.45
1:C:111:ASP:C	1:C:113:VAL:H	2.20	0.45
1:D:148:ALA:HB1	1:D:158:ILE:HD12	1.97	0.45
1:A:193:ARG:NH1	6:A:514:HOH:O	2.49	0.45
1:D:244:VAL:HG12	1:D:261:ILE:HG12	1.99	0.45
1:C:97:THR:HG21	1:C:166:ALA:HB2	1.99	0.45
1:D:122:ALA:O	1:D:126:VAL:HG23	2.17	0.45
1:C:117:ASN:OD1	2:C:401:PRP:O1B	2.33	0.44
1:C:263:ARG:HD3	1:C:336:TRP:CZ3	2.52	0.44
1:D:117:ASN:HB3	1:D:297:ASN:CG	2.38	0.44
1:C:33:ARG:HD2	1:C:40:LEU:HD23	2.00	0.44
1:D:72:LYS:O	1:D:73:ALA:HB3	2.17	0.44
4:C:405:17C:CAJ	4:C:405:17C:CAI	2.96	0.44
1:C:140:ALA:HB2	1:C:146:GLY:N	2.33	0.44
1:C:246:GLY:C	1:C:248:ASP:N	2.71	0.44
1:A:72:LYS:O	1:A:73:ALA:HB3	2.18	0.44
4:A:404:17C:CAI	4:A:404:17C:HAJ	2.47	0.43
1:C:157:ARG:HG2	1:C:160:LEU:HD21	2.00	0.43
4:A:404:17C:CAI	4:A:404:17C:CAJ	2.96	0.43
4:C:404:17C:CAJ	4:C:404:17C:HAI	2.49	0.43
1:B:208:LEU:HD23	1:B:234:PHE:CZ	2.54	0.43
1:C:97:THR:HG21	1:C:166:ALA:CB	2.49	0.43
1:A:244:VAL:HG12	1:A:261:ILE:HG12	2.01	0.43
4:D:403:17C:HAI	4:D:403:17C:HAJ	2.00	0.43
1:D:247:ASP:OD1	1:D:260:THR:HG23	2.19	0.42
1:B:58:ARG:HG3	1:D:195:GLU:HG2	2.00	0.42
1:C:94:PRO:O	1:C:97:THR:HB	2.19	0.42
1:C:285:GLN:HB2	1:C:288:GLN:HG3	2.02	0.42
1:C:65:PHE:CZ	1:C:69:MET:CE	3.03	0.42
1:D:187:ARG:HD2	4:D:402:17C:CAS	2.49	0.42
1:D:49:MET:O	1:D:53:MET:HG2	2.20	0.42
1:A:207:PRO:HB2	1:A:230:MET:CE	2.50	0.42
1:D:27:TRP:HB2	1:D:28:PRO:HD3	2.02	0.41
1:C:257:THR:HG23	1:C:258:THR:O	2.20	0.41
1:D:31:LEU:O	1:D:35:THR:HG23	2.21	0.41
1:C:193:ARG:HD3	1:C:202:PHE:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:GLN:HA	6:D:545:HOH:O	2.19	0.41
1:C:65:PHE:CE1	1:C:69:MET:HE3	2.56	0.41
1:B:304:VAL:HG21	1:B:312:VAL:HG12	2.03	0.41
1:A:60:ALA:O	1:C:196:ILE:HD11	2.21	0.41
1:B:179:ALA:HB3	1:B:180:PRO:HD3	2.02	0.41
1:C:148:ALA:HB1	1:C:158:ILE:CD1	2.49	0.40
1:D:62:ILE:HB	1:D:192:VAL:HG21	2.02	0.40
1:D:49:MET:HE2	1:D:82:LEU:HD22	2.04	0.40
1:B:263:ARG:CZ	1:B:272:LEU:HD11	2.51	0.40
1:D:49:MET:CE	1:D:82:LEU:HD22	2.50	0.40
1:C:72:LYS:O	1:C:73:ALA:HB3	2.20	0.40
1:B:52:ILE:HG21	1:B:189:ALA:HB2	2.03	0.40
1:C:72:LYS:O	1:C:73:ALA:CB	2.69	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	344/377 (91%)	338 (98%)	5 (2%)	1 (0%)	46	39
1	B	344/377 (91%)	335 (97%)	8 (2%)	1 (0%)	46	39
1	C	339/377 (90%)	324 (96%)	12 (4%)	3 (1%)	21	12
1	D	320/377 (85%)	309 (97%)	10 (3%)	1 (0%)	46	39
All	All	1347/1508 (89%)	1306 (97%)	35 (3%)	6 (0%)	39	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	247	ASP
1	A	73	ALA

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Mol	Chain	Res	Type
1	B	73	ALA
1	C	73	ALA
1	D	73	ALA
1	C	292	GLY

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	243/264 (92%)	243 (100%)	0	100	100
1	B	243/264 (92%)	243 (100%)	0	100	100
1	C	240/264 (91%)	237 (99%)	3 (1%)	76	77
1	D	232/264 (88%)	231 (100%)	1 (0%)	93	95
All	All	958/1056 (91%)	954 (100%)	4 (0%)	93	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	72	LYS
1	C	223	PHE
1	C	252	GLU
1	D	250	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	358	GLN
1	B	358	GLN
1	C	117	ASN
1	C	245	HIS
1	C	297	ASN
1	D	56	ASN
1	D	297	ASN

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Mol	Chain	Res	Type
1	D	358	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

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	PRP	A	401	3	19,22,22	1.62	3 (15%)	31,35,35	2.83	10 (32%)
4	17C	A	404	-	14,20,20	0.65	0	17,27,27	1.60	3 (17%)
2	PRP	B	401	3	19,22,22	1.90	6 (31%)	31,35,35	2.45	8 (25%)
4	17C	B	404	-	14,20,20	0.66	0	17,27,27	1.40	2 (11%)
2	PRP	C	401	3	19,22,22	1.74	4 (21%)	31,35,35	2.07	6 (19%)
4	17C	C	403	-	14,20,20	0.58	0	17,27,27	1.64	2 (11%)
4	17C	C	404	-	14,20,20	0.86	0	17,27,27	1.19	2 (11%)
4	17C	C	405	-	14,20,20	0.73	0	17,27,27	1.66	5 (29%)
5	DPO	D	401	-	8,8,8	4.30	4 (50%)	12,13,13	2.31	4 (33%)
4	17C	D	402	-	14,20,20	0.78	0	17,27,27	1.03	2 (11%)
4	17C	D	403	-	14,20,20	0.80	0	17,27,27	1.04	1 (5%)

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	PRP	A	401	3	-	0/16/33/33	0/1/1/1
4	17C	A	404	-	-	0/4/12/12	0/2/2/2
2	PRP	B	401	3	-	0/16/33/33	0/1/1/1
4	17C	B	404	-	-	0/4/12/12	0/2/2/2
2	PRP	C	401	3	-	0/16/33/33	0/1/1/1
4	17C	C	403	-	-	0/4/12/12	0/2/2/2
4	17C	C	404	-	-	0/4/12/12	0/2/2/2
4	17C	C	405	-	-	0/4/12/12	0/2/2/2
5	DPO	D	401	-	-	0/6/6/6	0/0/0/0
4	17C	D	402	-	-	0/4/12/12	0/2/2/2
4	17C	D	403	-	-	0/4/12/12	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PRP	PB-O3B	-2.18	1.46	1.54
2	B	401	PRP	PB-O3B	-2.10	1.47	1.54
2	B	401	PRP	P-O5	-2.01	1.53	1.60
2	B	401	PRP	C1-C2	2.02	1.55	1.52
2	C	401	PRP	PB-O2B	2.26	1.62	1.54
2	A	401	PRP	PB-O1B	2.84	1.60	1.51
2	C	401	PRP	PA-O1A	2.98	1.62	1.51
2	B	401	PRP	PA-O1A	2.99	1.62	1.51
2	C	401	PRP	PB-O1B	3.46	1.62	1.51
2	A	401	PRP	P-O1P	3.53	1.62	1.51
2	B	401	PRP	P-O1P	3.56	1.62	1.51
2	B	401	PRP	PB-O1B	3.63	1.63	1.51
2	C	401	PRP	P-O1P	3.64	1.63	1.51
5	D	401	DPO	P1-O2	4.57	1.59	1.51
5	D	401	DPO	P1-O1	5.65	1.62	1.51
5	D	401	DPO	P2-O7	6.37	1.63	1.51
5	D	401	DPO	P2-O6	6.78	1.63	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PRP	O4-C1-O1	-8.80	90.74	108.90
2	B	401	PRP	O4-C1-O1	-7.61	93.18	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	PRP	O4-C1-O1	-7.51	93.39	108.90
2	A	401	PRP	O4-C4-C3	-6.10	92.86	105.15
2	A	401	PRP	C2-C3-C4	-5.78	90.73	102.61
2	B	401	PRP	C2-C3-C4	-5.47	91.38	102.61
2	B	401	PRP	O4-C4-C3	-5.01	95.04	105.15
5	D	401	DPO	O2-P1-O1	-4.57	102.13	112.76
2	B	401	PRP	O2-C2-C3	-3.35	100.92	111.83
2	C	401	PRP	C5-C4-C3	-3.23	102.39	115.21
2	C	401	PRP	O4-C4-C3	-2.80	99.50	105.15
2	A	401	PRP	O2-C2-C3	-2.46	103.84	111.83
2	C	401	PRP	PA-O3A-PB	-2.34	124.81	132.67
4	C	405	17C	CAK-CAR-CAN	-2.17	116.89	120.23
2	A	401	PRP	O4-C1-C2	-2.10	101.83	104.78
4	D	403	17C	CAK-CAR-CAN	-2.05	117.07	120.23
4	A	404	17C	CAL-CAS-CAO	-2.04	117.09	120.23
2	A	401	PRP	O2P-P-O1P	-2.03	104.04	110.58
5	D	401	DPO	O2-P1-O4	-2.02	98.89	105.19
4	C	405	17C	CAE-CAG-CAK	-2.01	117.24	120.19
4	C	405	17C	CAI-CAP-CAR	-2.00	117.38	120.03
2	A	401	PRP	O2A-PA-O3A	2.06	114.43	105.09
4	D	402	17C	CAK-CAR-CAP	2.13	119.88	117.92
2	A	401	PRP	O3B-PB-O3A	2.31	115.59	105.09
2	B	401	PRP	O3P-P-O5	2.34	113.30	106.56
2	A	401	PRP	O3P-P-O5	2.37	113.40	106.56
2	B	401	PRP	O3B-PB-O3A	2.38	115.91	105.09
4	D	402	17C	CAL-CAS-CAQ	2.43	120.16	117.92
2	B	401	PRP	O4-C4-C5	2.61	118.67	109.32
2	C	401	PRP	O3P-P-O5	2.62	114.10	106.56
4	B	404	17C	CAL-CAS-CAQ	2.67	120.38	117.92
5	D	401	DPO	O6-P2-O4	2.72	113.64	105.19
4	C	404	17C	CAK-CAR-CAP	2.80	120.50	117.92
4	C	405	17C	CAK-CAR-CAP	3.05	120.73	117.92
4	C	404	17C	CAL-CAS-CAQ	3.11	120.78	117.92
4	C	403	17C	CAK-CAR-CAP	3.12	120.80	117.92
4	B	404	17C	CAK-CAR-CAP	3.13	120.81	117.92
4	A	404	17C	CAL-CAS-CAQ	3.34	121.00	117.92
4	C	405	17C	CAL-CAS-CAQ	3.40	121.06	117.92
5	D	401	DPO	O3-P1-O4	3.75	116.86	105.19
2	B	401	PRP	O1-C1-C2	3.78	113.41	106.67
4	A	404	17C	CAK-CAR-CAP	4.07	121.67	117.92
2	C	401	PRP	O1-C1-C2	4.41	114.53	106.67
4	C	403	17C	CAL-CAS-CAQ	4.45	122.03	117.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PRP	O1-C1-C2	6.63	118.49	106.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	17C	4	0
4	B	404	17C	2	0
2	C	401	PRP	4	0
4	C	404	17C	1	0
4	C	405	17C	4	0
4	D	402	17C	5	0
4	D	403	17C	5	0

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	346/377 (91%)	-0.16	7 (2%) 68 71	11, 19, 33, 49	0
1	B	346/377 (91%)	-0.20	5 (1%) 78 80	10, 20, 34, 47	0
1	C	343/377 (90%)	0.32	18 (5%) 31 35	15, 28, 56, 65	0
1	D	330/377 (87%)	0.21	15 (4%) 37 41	16, 27, 47, 66	0
All	All	1365/1508 (90%)	0.04	45 (3%) 50 54	10, 23, 46, 66	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	286	LEU	7.9
1	A	370	ILE	5.9
1	C	114	ASN	5.7
1	D	267	GLY	5.4
1	C	144	LEU	5.0
1	C	290	ALA	4.8
1	C	113	VAL	4.8
1	C	223	PHE	4.6
1	A	142	SER	4.5
1	D	223	PHE	4.4
1	D	292	GLY	4.1
1	C	142	SER	4.1
1	C	115	THR	3.9
1	C	141	ALA	3.8
1	C	116	VAL	3.4
1	C	333	ARG	3.3
1	A	144	LEU	3.2
1	C	112	GLY	3.1
1	C	296	ALA	2.9
1	A	141	ALA	2.9
1	D	110	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	140	ALA	2.7
1	C	332	SER	2.7
1	B	141	ALA	2.5
1	D	287	ASP	2.5
1	C	334	ALA	2.5
1	B	333	ARG	2.4
1	C	282	ALA	2.4
1	B	144	LEU	2.4
1	D	266	ALA	2.4
1	D	250	LEU	2.3
1	D	333	ARG	2.3
1	D	238	ARG	2.3
1	A	337	LEU	2.2
1	B	142	SER	2.2
1	A	334	ALA	2.2
1	C	299	ALA	2.2
1	A	332	SER	2.2
1	D	224	ALA	2.2
1	C	266	ALA	2.1
1	C	285	GLN	2.1
1	D	331	SER	2.1
1	D	289	LEU	2.1
1	D	294	ALA	2.1
1	B	370	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	17C	C	404	19/19	0.82	0.18	2.70	22,23,27,28	19
4	17C	D	403	19/19	0.81	0.21	2.67	20,23,25,25	19
5	DPO	D	401	9/9	0.84	0.21	2.05	18,21,24,24	9
4	17C	D	402	19/19	0.82	0.19	1.72	19,23,25,25	19
4	17C	C	403	19/19	0.90	0.13	1.29	23,28,34,37	0
2	PRP	C	401	22/22	0.91	0.20	0.73	31,34,36,37	22
2	PRP	B	401	22/22	0.97	0.13	0.60	15,20,22,22	13
4	17C	C	405	19/19	0.90	0.16	0.49	25,28,32,32	0
2	PRP	A	401	22/22	0.97	0.13	0.45	15,20,21,24	13
4	17C	B	404	19/19	0.94	0.10	0.08	21,23,27,28	0
4	17C	A	404	19/19	0.97	0.09	-0.22	17,19,26,27	0
3	MG	A	402	1/1	0.98	0.06	-	19,19,19,19	0
3	MG	C	402	1/1	0.91	0.07	-	17,17,17,17	1
3	MG	B	402	1/1	1.00	0.05	-	15,15,15,15	0
3	MG	B	403	1/1	0.98	0.06	-	22,22,22,22	0
3	MG	A	403	1/1	0.96	0.06	-	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.