



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 05:38 PM EDT

PDB ID : 3CC9
Title : Crystal structure of Plasmodium vivax putative polyprenyl pyrophosphate synthase in complex with geranylgeranyl diphosphate
Authors : Wernimont, A.K.; Dunford, J.; Lew, J.; Zhao, Y.; Kozieradzki, I.; Cossar, D.; Schapira, M.; Bochkarev, A.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Hui, R.; Artz, J.D.; Structural Genomics Consortium (SGC)
Deposited on : unknown
Resolution : 2.30 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

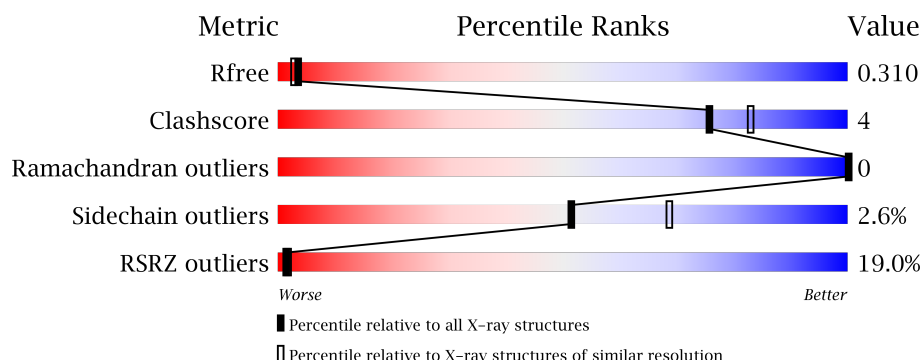
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	396	<div> <div>13%</div> <div> <div></div> <div>74%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	396	<div> <div>13%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div></div> <div>10%</div> </div> </div>
1	C	396	<div> <div>25%</div> <div> <div></div> <div>76%</div> <div>8%</div> <div></div> <div>16%</div> </div> </div>
1	D	396	<div> <div>15%</div> <div> <div></div> <div>79%</div> <div>6%</div> <div>•</div> <div>15%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11221 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 Putative farnesyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	1	0
			2764	1793	439	517	15			
1	B	358	Total	C	N	O	S	0	2	0
			2885	1873	462	535	15			
1	C	332	Total	C	N	O	S	0	0	0
			2578	1663	420	481	14			
1	D	337	Total	C	N	O	S	0	0	0
			2639	1702	423	499	15			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP A5K4U6
A	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
A	3	SER	-	EXPRESSION TAG	UNP A5K4U6
A	4	SER	-	EXPRESSION TAG	UNP A5K4U6
A	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	11	SER	-	EXPRESSION TAG	UNP A5K4U6
A	12	SER	-	EXPRESSION TAG	UNP A5K4U6
A	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
A	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
A	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
A	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
A	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
A	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
A	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
A	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
A	21	GLY	-	EXPRESSION TAG	UNP A5K4U6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	134	MET	THR	SEE REMARK 999	UNP A5K4U6
A	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
B	1	MET	-	EXPRESSION TAG	UNP A5K4U6
B	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	3	SER	-	EXPRESSION TAG	UNP A5K4U6
B	4	SER	-	EXPRESSION TAG	UNP A5K4U6
B	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	11	SER	-	EXPRESSION TAG	UNP A5K4U6
B	12	SER	-	EXPRESSION TAG	UNP A5K4U6
B	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
B	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
B	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
B	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
B	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
B	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
B	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
B	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	134	MET	THR	SEE REMARK 999	UNP A5K4U6
B	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
C	1	MET	-	EXPRESSION TAG	UNP A5K4U6
C	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	3	SER	-	EXPRESSION TAG	UNP A5K4U6
C	4	SER	-	EXPRESSION TAG	UNP A5K4U6
C	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	11	SER	-	EXPRESSION TAG	UNP A5K4U6
C	12	SER	-	EXPRESSION TAG	UNP A5K4U6
C	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
C	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
C	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
C	17	LEU	-	EXPRESSION TAG	UNP A5K4U6

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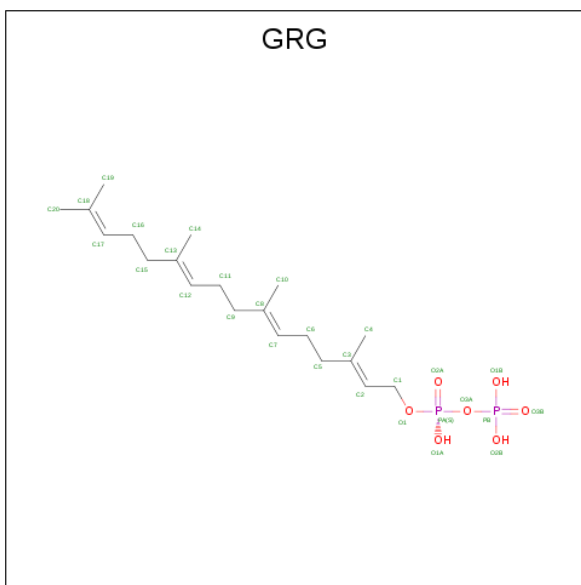
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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
C	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
C	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
C	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	134	MET	THR	SEE REMARK 999	UNP A5K4U6
C	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
D	1	MET	-	EXPRESSION TAG	UNP A5K4U6
D	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	3	SER	-	EXPRESSION TAG	UNP A5K4U6
D	4	SER	-	EXPRESSION TAG	UNP A5K4U6
D	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	11	SER	-	EXPRESSION TAG	UNP A5K4U6
D	12	SER	-	EXPRESSION TAG	UNP A5K4U6
D	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
D	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
D	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
D	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
D	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
D	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
D	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
D	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	134	MET	THR	SEE REMARK 999	UNP A5K4U6
D	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is GERANYLGERANYL DIPHOSPHATE (three-letter code: GRG) (formula: C₂₀H₃₆O₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 29	C 20	O 7	P 2	0	0
3	B	1	Total 29	C 20	O 7	P 2	0	0
3	C	1	Total 27	C 18	O 7	P 2	0	0
3	D	1	Total 29	C 20	O 7	P 2	0	0

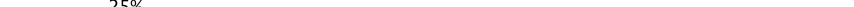
- Molecule 4 is water.

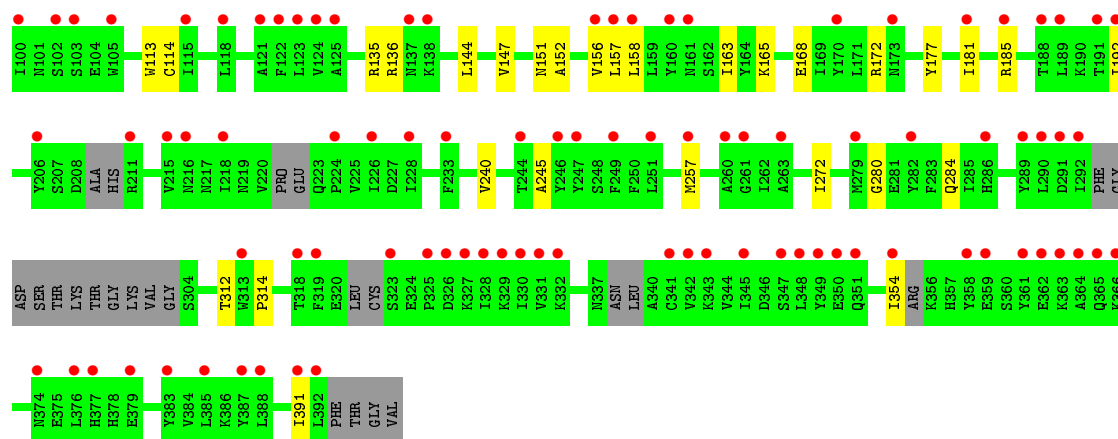
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	75	Total O 75 75	0	0
4	B	83	Total O 83 83	0	0
4	C	47	Total O 47 47	0	0
4	D	35	Total O 35 35	0	0

These plots are drawn for all protein, RNA and DNA 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.

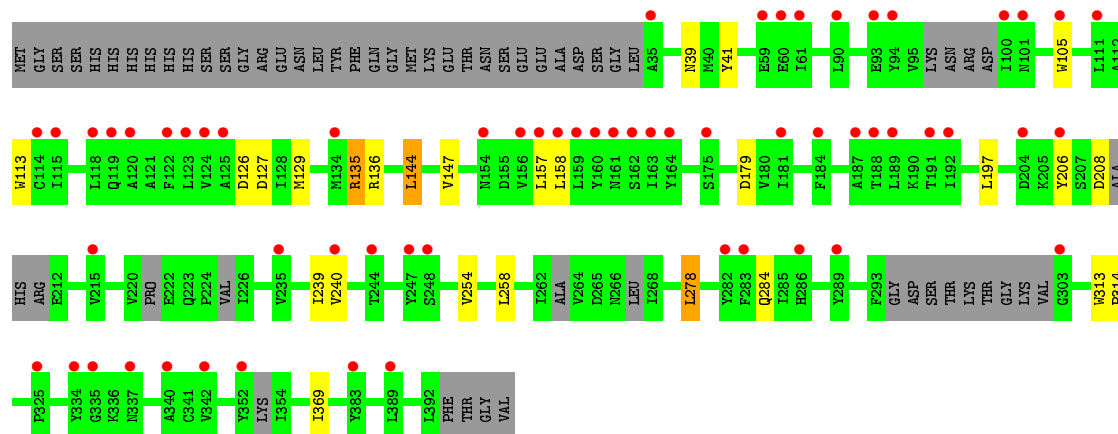
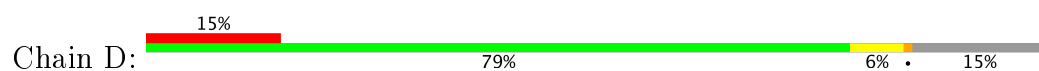
- Chain A:
-
- Sequence logo for Chain A, showing amino acid conservation across 100 positions. The y-axis represents information content in bits, ranging from 0 to 1.0. The x-axis shows positions 1 to 100. A color scale at the top indicates conservation levels: 13% (red), 74% (green), 11% (yellow), and 13% (grey). Amino acids are labeled at the top of each position, with some positions having multiple labels. Red dots above the labels indicate specific amino acids present at that position.

- Chain B:
-
- 13% 84% 7% 10%
- MET GLY SER SER HIS HIS HIS HIS HIS HIS ARG GLU ASN LEU PHE GLN MET LYS GLU THR ASN SER GLU GLU ALA ASP SER SER LEU A35 F36 F37 Y41 Y69 A112 W113 C114 I115 E116 I117 L118 Q119 A120 A121 F122 L123 V124 A125 I128 M129 L144 L152 V153 V156 L157 L158 L159 N160 N161 S162 I163 Y164 K165 L166 L167 E168 R172 R184 T186 L189 K190 T191 I192 Q195 H196 L197 K205 Y206 N217 N218 N219 VAL P221 P224 V225 T226 Y236 V240 K243 T244 Y247 S248 L251 P252 C255 T262 VAL D265 Q284 V302 GLY S304 Q307 L311 P314 P325 I328 V331 A340 V344 I354 A364 A367 S371 A372 L376 V396

- Chain C: 



• Molecule 1: Putative farnesyl pyrophosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.09Å 108.98Å 141.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.61 – 2.30 34.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.61-2.30) 99.7 (34.40-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.296 0.273 , 0.310	Depositor DCC
R_{free} test set	3721 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11221	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GRG, NA

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	0.36	0/2821	0.54	3/3829 (0.1%)
1	B	0.38	0/2952	0.53	2/3999 (0.1%)
1	C	0.33	0/2626	0.46	0/3569
1	D	0.34	0/2687	0.49	0/3644
All	All	0.36	0/11086	0.51	5/15041 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	LEU	CA-CB-CG	-5.83	101.88	115.30
1	A	84	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	123	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	157	LEU	CA-CB-CG	-5.41	102.85	115.30
1	B	123	LEU	CA-CB-CG	5.29	127.46	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2764	0	2595	31	0
1	B	2885	0	2749	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2578	0	2319	17	0
1	D	2639	0	2417	14	0
2	A	1	0	0	0	0
3	A	29	0	21	2	0
3	B	29	0	21	2	0
3	C	27	0	15	0	0
3	D	29	0	23	1	0
4	A	75	0	0	0	0
4	B	83	0	0	1	0
4	C	47	0	0	1	0
4	D	35	0	0	0	0
All	All	11221	0	10160	75	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 4.

All (75) 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:161:ASN:HB3	1:B:189:LEU:HD11	1.71	0.73
1:A:161:ASN:HB3	1:B:189:LEU:CD1	2.19	0.72
1:A:157:LEU:HD22	3:B:501:GRG:H203	1.73	0.71
1:D:127:ASP:OD2	1:D:135:ARG:HG3	1.92	0.69
1:A:84:ARG:NH1	3:A:501:GRG:O2A	2.25	0.68
1:A:168:GLU:O	1:A:172:ARG:HB2	1.95	0.67
1:A:59[A]:GLU:H	1:A:59[A]:GLU:CD	1.98	0.67
1:A:129:MET:CE	1:A:195:GLN:HE21	2.09	0.64
1:D:240:VAL:HG22	1:D:284:GLN:HG2	1.77	0.64
1:B:205:LYS:HG3	1:B:206:TYR:HD2	1.63	0.62
1:B:168:GLU:O	1:B:172:ARG:HB2	1.99	0.62
1:A:240:VAL:HG22	1:A:284:GLN:HG2	1.84	0.60
1:B:240:VAL:HG22	1:B:284:GLN:HG2	1.84	0.58
1:A:91:ILE:O	1:A:95:VAL:HG22	2.05	0.56
1:A:91:ILE:HD13	1:A:253:ILE:HA	1.87	0.56
1:A:240:VAL:HG11	1:A:281:GLU:HA	1.88	0.56
1:C:257:MET:SD	1:C:272:ILE:HD13	2.46	0.55
1:A:145:LYS:HD2	1:B:217:ASN:ND2	2.21	0.54
1:C:41:TYR:HB2	1:C:113:TRP:CZ2	2.43	0.54
1:D:41:TYR:HB2	1:D:113:TRP:CZ2	2.43	0.54
1:C:192:ILE:HG21	1:D:158:LEU:HB2	1.90	0.53
1:B:205:LYS:HG3	1:B:206:TYR:CD2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:GLN:HE21	1:B:243:LYS:HD2	1.75	0.51
1:B:41:TYR:HB2	1:B:113:TRP:CZ2	2.46	0.51
1:C:168:GLU:O	1:C:172:ARG:HB3	2.10	0.51
1:C:312:THR:HB	1:C:314:PRO:HD2	1.92	0.51
1:C:136:ARG:HD2	4:C:528:HOH:O	2.11	0.50
1:A:91:ILE:HG13	1:A:384:VAL:HG11	1.92	0.50
1:A:129:MET:HE1	1:A:195:GLN:HE21	1.77	0.49
1:A:84:ARG:HD3	1:A:248:SER:HA	1.94	0.49
1:A:254:VAL:O	1:A:258:LEU:HB2	2.12	0.49
1:C:240:VAL:HG22	1:C:284:GLN:HG2	1.95	0.49
1:D:136:ARG:HD2	3:D:501:GRG:O2B	2.13	0.49
1:B:226:ILE:HD11	1:B:331:VAL:HG22	1.95	0.49
1:D:278:LEU:HB3	1:D:369:ILE:HG12	1.94	0.48
3:A:501:GRG:H203	1:B:157:LEU:HD22	1.95	0.48
1:C:245:ALA:HB2	1:C:280:GLY:HA3	1.96	0.48
1:A:205:LYS:HG3	1:A:206:TYR:HD2	1.79	0.48
1:C:64:HIS:CD2	1:D:206:TYR:HA	2.48	0.47
1:D:254:VAL:O	1:D:258:LEU:HB2	2.13	0.47
1:A:41:TYR:HB2	1:A:113:TRP:CZ2	2.50	0.47
1:D:144:LEU:HB2	1:D:147:VAL:HG12	1.97	0.47
1:A:202:PHE:HB3	1:A:225:VAL:O	2.15	0.46
1:A:312:THR:HB	1:A:314:PRO:HD2	1.98	0.46
1:C:69:TYR:CE1	1:C:158:LEU:HD22	2.49	0.46
1:C:69:TYR:CD1	1:C:158:LEU:HD22	2.51	0.46
1:B:340:ALA:O	1:B:344:VAL:HG23	2.16	0.46
1:D:126:ASP:HA	1:D:129:MET:HE3	1.98	0.45
1:B:69:TYR:CE1	1:B:158:LEU:HD22	2.52	0.44
1:C:314:PRO:HB3	1:C:354:ILE:HG21	1.99	0.44
1:B:314:PRO:HB3	1:B:354:ILE:HG21	2.00	0.44
1:C:152:ALA:O	1:C:156:VAL:HG23	2.17	0.44
1:D:144:LEU:HB2	1:D:147:VAL:CG1	2.47	0.44
1:B:69:TYR:CD1	1:B:158:LEU:HD22	2.53	0.44
1:C:177:TYR:CZ	1:C:181:ILE:HD11	2.53	0.44
1:A:152:ALA:O	1:A:156:VAL:HG23	2.18	0.43
1:B:195:GLN:CG	3:B:501:GRG:HC91	2.49	0.43
1:C:114:CYS:HB3	1:C:163:ILE:HG23	2.00	0.43
1:A:88:VAL:HG21	1:A:115:ILE:HD12	2.01	0.43
1:A:69:TYR:CD1	1:A:158:LEU:HD22	2.54	0.43
1:A:91:ILE:CD1	1:A:253:ILE:HG12	2.49	0.42
1:B:236:TYR:CZ	1:B:240:VAL:HG21	2.54	0.42
1:A:223:GLN:HA	1:A:224:PRO:HD3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:VAL:O	1:C:151:ASN:HB2	2.19	0.42
1:A:197:LEU:O	1:A:201:ILE:HB	2.19	0.42
1:D:313:TRP:HB3	1:D:314:PRO:HD3	2.01	0.42
1:A:285:ILE:HD12	1:A:361:TYR:CZ	2.55	0.41
1:A:126:ASP:HA	1:A:129:MET:HE3	2.03	0.41
1:A:69:TYR:O	1:A:73:PHE:HD2	2.03	0.41
1:C:391:ILE:O	1:C:391:ILE:HG22	2.21	0.41
1:A:123:LEU:HG	1:A:135:ARG:HG2	2.03	0.40
1:D:197:LEU:HB3	1:D:239:ILE:HG12	2.03	0.40
1:D:179:ASP:HB3	1:D:258:LEU:HD21	2.02	0.40
1:B:224:PRO:HA	4:B:581:HOH:O	2.21	0.40
1:A:235:VAL:O	1:A:238:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	335/396 (85%)	329 (98%)	6 (2%)	0	100	100
1	B	352/396 (89%)	341 (97%)	11 (3%)	0	100	100
1	C	316/396 (80%)	308 (98%)	8 (2%)	0	100	100
1	D	319/396 (81%)	308 (97%)	11 (3%)	0	100	100
All	All	1322/1584 (84%)	1286 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/357 (78%)	266 (96%)	11 (4%)	36	50
1	B	294/357 (82%)	290 (99%)	4 (1%)	71	85
1	C	235/357 (66%)	228 (97%)	7 (3%)	46	63
1	D	255/357 (71%)	248 (97%)	7 (3%)	50	67
All	All	1061/1428 (74%)	1032 (97%)	29 (3%)	51	67

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	PHE
1	A	59[A]	GLU
1	A	59[B]	GLU
1	A	65	ILE
1	A	144	LEU
1	A	157	LEU
1	A	185	ARG
1	A	238	ASN
1	A	258	LEU
1	A	264	VAL
1	A	321	LEU
1	B	144	LEU
1	B	157	LEU
1	B	262	ILE
1	B	307	GLN
1	C	39	ASN
1	C	64	HIS
1	C	135	ARG
1	C	144	LEU
1	C	157	LEU
1	C	165	LYS
1	C	185	ARG
1	D	39	ASN
1	D	105	TRP
1	D	135	ARG
1	D	144	LEU
1	D	157	LEU
1	D	208	ASP

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Mol	Chain	Res	Type
1	D	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	ASN
1	C	64	HIS
1	C	82	ASN
1	C	173	ASN
1	D	195	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
3	GRG	A	501	-	27,28,28	2.87	7 (25%)	30,37,37	7.31	12 (40%)
3	GRG	B	501	-	27,28,28	2.83	8 (29%)	30,37,37	6.87	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GRG	C	501	-	25,26,28	2.96	7 (28%)	27,34,37	8.00	11 (40%)
3	GRG	D	501	-	27,28,28	2.82	8 (29%)	30,37,37	6.51	9 (30%)

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
3	GRG	A	501	-	-	1/31/31/31	0/0/0/0
3	GRG	B	501	-	-	2/31/31/31	0/0/0/0
3	GRG	C	501	-	-	0/29/29/31	0/0/0/0
3	GRG	D	501	-	-	0/31/31/31	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	GRG	C1-C2	-7.54	1.25	1.49
3	A	501	GRG	C1-C2	-7.41	1.26	1.49
3	C	501	GRG	C11-C12	-7.18	1.26	1.50
3	C	501	GRG	C6-C7	-7.14	1.26	1.50
3	D	501	GRG	C11-C12	-7.13	1.26	1.50
3	A	501	GRG	C11-C12	-7.10	1.26	1.50
3	B	501	GRG	C6-C7	-7.04	1.26	1.50
3	D	501	GRG	C1-C2	-7.02	1.27	1.49
3	B	501	GRG	C1-C2	-6.94	1.27	1.49
3	A	501	GRG	C6-C7	-6.88	1.27	1.50
3	B	501	GRG	C11-C12	-6.70	1.27	1.50
3	D	501	GRG	C6-C7	-6.53	1.28	1.50
3	B	501	GRG	C16-C17	-6.51	1.28	1.50
3	D	501	GRG	C16-C17	-6.06	1.29	1.50
3	A	501	GRG	C16-C17	-6.03	1.29	1.50
3	C	501	GRG	C16-C17	-5.23	1.26	1.49
3	C	501	GRG	C2-C3	-2.82	1.25	1.33
3	C	501	GRG	C7-C8	-2.80	1.26	1.33
3	D	501	GRG	C12-C13	-2.79	1.26	1.33
3	C	501	GRG	C12-C13	-2.76	1.26	1.33
3	D	501	GRG	C2-C3	-2.75	1.26	1.33
3	A	501	GRG	C7-C8	-2.72	1.26	1.33
3	A	501	GRG	C12-C13	-2.72	1.26	1.33
3	D	501	GRG	C7-C8	-2.65	1.26	1.33
3	A	501	GRG	C2-C3	-2.65	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	GRG	C7-C8	-2.60	1.26	1.33
3	B	501	GRG	C2-C3	-2.57	1.26	1.33
3	B	501	GRG	C12-C13	-2.41	1.26	1.33
3	D	501	GRG	O1-C1	2.19	1.46	1.43
3	B	501	GRG	O1-C1	2.23	1.46	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	GRG	C4-C3-C2	-2.28	117.61	123.69
3	B	501	GRG	C10-C8-C7	-2.27	117.63	123.69
3	A	501	GRG	C10-C8-C7	-2.06	118.19	123.69
3	A	501	GRG	C14-C13-C12	-2.05	118.23	123.69
3	C	501	GRG	O1-C1-C2	2.06	118.88	109.73
3	A	501	GRG	C9-C11-C12	2.21	119.55	111.97
3	A	501	GRG	O1-C1-C2	2.23	119.62	109.73
3	D	501	GRG	C9-C11-C12	2.35	120.03	111.97
3	C	501	GRG	C9-C11-C12	2.52	120.63	111.97
3	C	501	GRG	C5-C6-C7	2.53	120.66	111.97
3	B	501	GRG	C14-C13-C15	2.57	119.75	115.29
3	B	501	GRG	C9-C11-C12	2.72	121.28	111.97
3	D	501	GRG	C10-C8-C9	2.73	120.03	115.29
3	C	501	GRG	C10-C8-C9	2.75	120.06	115.29
3	A	501	GRG	C10-C8-C9	2.85	120.23	115.29
3	B	501	GRG	C10-C8-C9	2.92	120.36	115.29
3	D	501	GRG	C15-C16-C17	3.16	122.79	111.97
3	A	501	GRG	C14-C13-C15	3.30	121.01	115.29
3	C	501	GRG	C14-C13-C15	3.34	121.08	115.29
3	D	501	GRG	C14-C13-C15	3.43	121.23	115.29
3	A	501	GRG	C4-C3-C5	3.43	121.23	115.29
3	D	501	GRG	C4-C3-C5	3.44	121.26	115.29
3	B	501	GRG	C15-C16-C17	3.50	123.97	111.97
3	C	501	GRG	C15-C16-C17	3.64	120.67	112.24
3	A	501	GRG	C15-C16-C17	3.66	124.54	111.97
3	B	501	GRG	C4-C3-C5	3.89	122.03	115.29
3	C	501	GRG	C4-C3-C5	4.07	122.36	115.29
3	C	501	GRG	C16-C17-C18	6.79	172.04	126.70
3	A	501	GRG	C16-C17-C18	9.47	161.60	127.80
3	D	501	GRG	C16-C17-C18	9.53	161.79	127.80
3	B	501	GRG	C16-C17-C18	10.98	166.98	127.80
3	D	501	GRG	C6-C7-C8	15.07	165.54	127.68
3	A	501	GRG	C6-C7-C8	16.71	169.65	127.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	GRG	C6-C7-C8	17.70	172.14	127.68
3	A	501	GRG	C11-C12-C13	18.03	172.97	127.68
3	B	501	GRG	C11-C12-C13	18.32	173.70	127.68
3	D	501	GRG	C11-C12-C13	19.00	175.41	127.68
3	C	501	GRG	C11-C12-C13	19.05	175.53	127.68
3	C	501	GRG	C6-C7-C8	20.51	179.21	127.68
3	D	501	GRG	C1-C2-C3	22.78	167.91	125.96
3	B	501	GRG	C1-C2-C3	23.77	169.74	125.96
3	C	501	GRG	C1-C2-C3	28.52	178.49	125.96
3	A	501	GRG	C1-C2-C3	28.81	179.02	125.96

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GRG	C1-C2-C3-C4
3	B	501	GRG	C1-C2-C3-C4
3	B	501	GRG	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GRG	2	0
3	B	501	GRG	2	0
3	D	501	GRG	1	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	344/396 (86%)	0.74	50 (14%) 3 4	45, 57, 70, 76	1 (0%)
1	B	358/396 (90%)	0.75	52 (14%) 3 4	45, 57, 70, 80	0
1	C	332/396 (83%)	1.33	98 (29%) 1 0	49, 65, 77, 91	0
1	D	337/396 (85%)	0.91	61 (18%) 1 2	50, 61, 77, 110	0
All	All	1371/1584 (86%)	0.93	261 (19%) 1 2	45, 59, 75, 110	1 (0%)

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	TYR	7.1
1	D	206	TYR	6.8
1	C	330	ILE	6.3
1	C	354	ILE	5.7
1	C	325	PRO	5.6
1	C	290	LEU	5.5
1	C	342	VAL	5.4
1	A	394	THR	5.2
1	A	158	LEU	5.0
1	C	94	TYR	5.0
1	B	160	TYR	4.9
1	C	383	TYR	4.9
1	A	157	LEU	4.9
1	C	318	THR	4.9
1	C	341	CYS	4.8
1	C	358	TYR	4.8
1	C	102	SER	4.8
1	D	191	THR	4.6
1	D	105	TRP	4.6
1	B	192	ILE	4.6
1	C	192	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	215	VAL	4.5
1	D	192	ILE	4.4
1	C	313	TRP	4.4
1	C	328	ILE	4.3
1	D	157	LEU	4.3
1	C	345	ILE	4.2
1	C	170	TYR	4.1
1	B	191	THR	4.1
1	A	395	GLY	4.1
1	C	361	TYR	4.0
1	D	160	TYR	4.0
1	A	192	ILE	4.0
1	C	347	SER	4.0
1	C	291	ASP	4.0
1	D	134	MET	3.9
1	B	124	VAL	3.9
1	B	158	LEU	3.9
1	D	158	LEU	3.9
1	D	101	ASN	3.8
1	C	218	ILE	3.8
1	D	162	SER	3.8
1	C	319	PHE	3.8
1	B	118	LEU	3.8
1	A	156	VAL	3.8
1	C	326	ASP	3.7
1	B	120	ALA	3.7
1	A	338	ASN	3.6
1	B	157	LEU	3.6
1	C	379	GLU	3.6
1	C	157	LEU	3.6
1	C	331	VAL	3.6
1	C	391	ILE	3.5
1	A	160	TYR	3.5
1	C	188	THR	3.5
1	D	159	LEU	3.5
1	D	175	SER	3.5
1	C	363	LYS	3.5
1	A	293	PHE	3.5
1	C	115	ILE	3.4
1	A	154	ASN	3.4
1	D	115	ILE	3.4
1	C	365	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	323	SER	3.4
1	B	247	TYR	3.4
1	A	117	ILE	3.4
1	A	124	VAL	3.3
1	A	153	VAL	3.3
1	A	159	LEU	3.3
1	A	355	ARG	3.3
1	B	117	ILE	3.3
1	A	121	ALA	3.3
1	A	36	PHE	3.3
1	A	122	PHE	3.3
1	A	319	PHE	3.3
1	C	244	THR	3.3
1	C	121	ALA	3.2
1	A	102	SER	3.2
1	B	115	ILE	3.2
1	C	158	LEU	3.2
1	D	122	PHE	3.2
1	D	383	TYR	3.2
1	B	156	VAL	3.2
1	D	118	LEU	3.2
1	A	391	ILE	3.1
1	B	122	PHE	3.1
1	C	376	LEU	3.1
1	A	105	TRP	3.1
1	D	244	THR	3.1
1	C	377	HIS	3.1
1	C	122	PHE	3.1
1	A	118	LEU	3.1
1	A	339	LEU	3.1
1	A	393	PHE	3.1
1	B	188	THR	3.0
1	D	352	TYR	3.0
1	C	359	GLU	3.0
1	D	334	TYR	3.0
1	A	220	VAL	3.0
1	C	92	TYR	3.0
1	D	120	ALA	3.0
1	D	342	VAL	3.0
1	A	189	LEU	3.0
1	C	161	ASN	3.0
1	B	163	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	105	TRP	2.9
1	C	75	TYR	2.9
1	B	153	VAL	2.8
1	D	163	ILE	2.8
1	D	100	ILE	2.8
1	D	184	PHE	2.8
1	A	123	LEU	2.8
1	D	94	TYR	2.8
1	A	194	GLY	2.8
1	A	164	TYR	2.8
1	C	189	LEU	2.8
1	C	279	MET	2.8
1	C	350	GLU	2.8
1	B	248	SER	2.7
1	A	115	ILE	2.7
1	C	86	ILE	2.7
1	B	123	LEU	2.7
1	C	351	GLN	2.7
1	B	244	THR	2.7
1	B	252	PRO	2.7
1	D	240	VAL	2.7
1	B	164	TYR	2.7
1	A	114	CYS	2.7
1	C	233	PHE	2.7
1	D	114	CYS	2.7
1	D	235	VAL	2.7
1	B	189	LEU	2.7
1	D	123	LEU	2.7
1	D	337	ASN	2.7
1	B	152	ALA	2.6
1	C	124	VAL	2.6
1	A	341	CYS	2.6
1	B	396	VAL	2.6
1	D	164	TYR	2.6
1	D	248	SER	2.6
1	A	125	ALA	2.6
1	C	260	ALA	2.6
1	C	263	ALA	2.6
1	B	162	SER	2.6
1	C	40	MET	2.6
1	C	387	TYR	2.6
1	D	156	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	161	ASN	2.6
1	B	125	ALA	2.6
1	A	193	ILE	2.6
1	D	154	ASN	2.6
1	D	188	THR	2.6
1	D	124	VAL	2.6
1	B	37	PHE	2.5
1	C	125	ALA	2.5
1	C	332	LYS	2.5
1	C	343	LYS	2.5
1	D	90	LEU	2.5
1	D	189	LEU	2.5
1	B	161	ASN	2.5
1	A	251	LEU	2.5
1	D	247	TYR	2.5
1	A	163	ILE	2.5
1	B	129	MET	2.5
1	A	120	ALA	2.5
1	B	262	ILE	2.5
1	C	348	LEU	2.5
1	C	185	ARG	2.4
1	C	39	ASN	2.4
1	B	328	ILE	2.4
1	D	282	TYR	2.4
1	A	38	ARG	2.4
1	C	366	LYS	2.4
1	D	93	GLU	2.4
1	C	362	GLU	2.4
1	A	162	SER	2.4
1	B	197	LEU	2.4
1	B	372	ALA	2.4
1	A	191	THR	2.4
1	B	159	LEU	2.4
1	D	125	ALA	2.4
1	D	204	ASP	2.3
1	A	247	TYR	2.3
1	C	160	TYR	2.3
1	C	247	TYR	2.3
1	C	123	LEU	2.3
1	D	35	ALA	2.3
1	D	181	ILE	2.3
1	D	289	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	243	LYS	2.3
1	A	161	ASN	2.3
1	C	329	LYS	2.3
1	C	228	ILE	2.3
1	D	61	ILE	2.3
1	B	311	LEU	2.3
1	C	118	LEU	2.3
1	B	371	SER	2.3
1	C	216	ASN	2.3
1	C	385	LEU	2.3
1	C	327	LYS	2.3
1	B	302	VAL	2.3
1	A	245	ALA	2.3
1	A	340	ALA	2.3
1	B	166	LEU	2.3
1	C	54	GLU	2.3
1	C	173	ASN	2.3
1	A	182	ALA	2.3
1	B	121	ALA	2.3
1	B	184	PHE	2.2
1	C	249	PHE	2.2
1	A	188	THR	2.2
1	C	211	ARG	2.2
1	B	251	LEU	2.2
1	B	240	VAL	2.2
1	B	128	ILE	2.2
1	B	376	LEU	2.2
1	C	251	LEU	2.2
1	D	286	HIS	2.2
1	C	246	TYR	2.2
1	B	114	CYS	2.2
1	D	60	GLU	2.2
1	C	392	LEU	2.2
1	C	224	PRO	2.2
1	C	191	THR	2.2
1	D	340	ALA	2.2
1	D	325	PRO	2.2
1	D	187	ALA	2.2
1	C	100	ILE	2.2
1	B	367	ALA	2.1
1	D	59	GLU	2.1
1	B	325	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	289	TYR	2.1
1	C	364	ALA	2.1
1	C	181	ILE	2.1
1	C	374	ASN	2.1
1	D	111	LEU	2.1
1	A	250	PHE	2.1
1	B	112	ALA	2.1
1	B	364	ALA	2.1
1	A	155	ASP	2.1
1	C	282	TYR	2.1
1	C	261	GLY	2.1
1	A	289	TYR	2.1
1	D	283	PHE	2.1
1	D	303	GLY	2.1
1	C	137	ASN	2.1
1	B	255	CYS	2.1
1	C	103	SER	2.1
1	C	156	VAL	2.1
1	C	206	TYR	2.1
1	C	292	ILE	2.0
1	D	389	LEU	2.0
1	D	335	GLY	2.0
1	D	215	VAL	2.0
1	C	138	LYS	2.0
1	C	257	MET	2.0
1	C	286	HIS	2.0
1	C	226	ILE	2.0
1	C	388	LEU	2.0
1	B	195	GLN	2.0
1	D	119	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

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
3	GRG	D	501	29/29	0.93	0.37	1.56	38,49,65,65	20
3	GRG	C	501	27/29	0.94	0.22	-0.16	67,70,74,75	0
3	GRG	B	501	29/29	0.96	0.21	-0.79	43,49,51,52	0
3	GRG	A	501	29/29	0.96	0.17	-1.01	43,48,54,55	0
2	NA	A	502	1/1	0.94	0.15	-1.79	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.