



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:19 AM GMT

PDB ID : 3LNM  
Title : F233W mutant of the Kv2.1 paddle-Kv1.2 chimera channel  
Authors : Tao, X.; Lee, A.; Limapichat, W.; Dougherty, D.A.; MacKinnon, R.  
Deposited on : 2010-02-02  
Resolution : 2.90 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](mailto: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.

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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

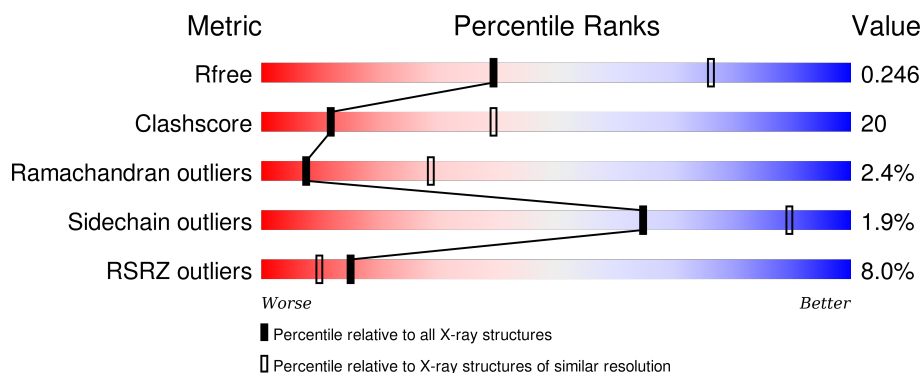
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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  $\geq 3$ , 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	333	<div> <div></div> <div>76% 21% ..</div> </div>
1	C	333	<div> <div></div> <div>71% 26% ..</div> </div>
2	B	514	<div> <div>10%</div> <div>46% 27% • 24%</div> </div>
2	D	514	<div> <div>11%</div> <div>31% 28% • 38%</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	PGW	B	601	-	-	-	X
4	PGW	B	605	-	-	-	X
4	PGW	B	606	-	-	-	X
4	PGW	B	608	-	-	-	X
4	PGW	B	609	-	-	-	X
4	PGW	B	611	-	-	-	X
4	PGW	D	601	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11308 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 Voltage-gated potassium channel subunit beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2556	1627	443	470	16			
1	C	326	Total	C	N	O	S	0	0	0
			2556	1627	443	470	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	INITIATING METHIONINE	UNP P62483
C	35	MET	-	INITIATING METHIONINE	UNP P62483

- Molecule 2 is a protein called F233W mutant of the Kv2.1 paddle-Kv1.2 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	389	Total	C	N	O	S	0	0	0
			3116	2038	510	554	14			
2	D	318	Total	C	N	O	S	0	0	0
			2584	1702	419	451	12			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	EXPRESSION TAG	UNP P63142
B	-17	ALA	-	EXPRESSION TAG	UNP P63142
B	-16	HIS	-	EXPRESSION TAG	UNP P63142
B	-15	HIS	-	EXPRESSION TAG	UNP P63142
B	-14	HIS	-	EXPRESSION TAG	UNP P63142
B	-13	HIS	-	EXPRESSION TAG	UNP P63142
B	-12	HIS	-	EXPRESSION TAG	UNP P63142
B	-11	HIS	-	EXPRESSION TAG	UNP P63142
B	-10	HIS	-	EXPRESSION TAG	UNP P63142
B	-9	HIS	-	EXPRESSION TAG	UNP P63142

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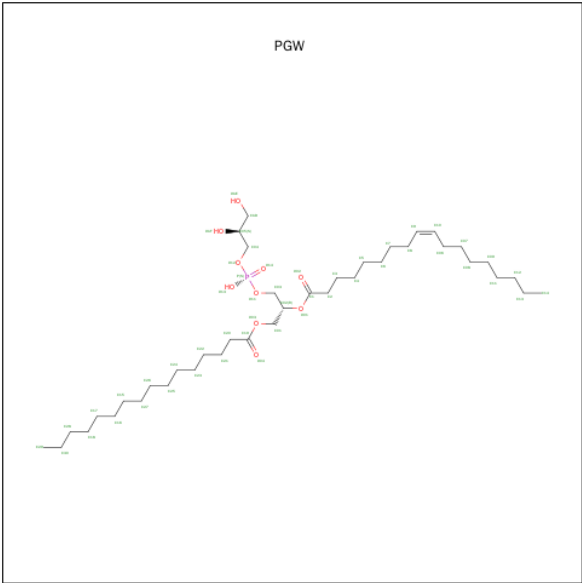
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	EXPRESSION TAG	UNP P63142
B	-7	HIS	-	EXPRESSION TAG	UNP P63142
B	-6	GLY	-	EXPRESSION TAG	UNP P63142
B	-5	LEU	-	EXPRESSION TAG	UNP P63142
B	-4	VAL	-	EXPRESSION TAG	UNP P63142
B	-3	PRO	-	EXPRESSION TAG	UNP P63142
B	-2	ARG	-	EXPRESSION TAG	UNP P63142
B	-1	GLY	-	EXPRESSION TAG	UNP P63142
B	0	SER	-	EXPRESSION TAG	UNP P63142
B	31	SER	CYS	ENGINEERED	UNP P63142
B	32	SER	CYS	ENGINEERED	UNP P63142
B	207	GLN	ASN	ENGINEERED	UNP P63142
B	233	TRP	PHE	ENGINEERED	UNP P63142
B	431	SER	CYS	ENGINEERED	UNP P63142
B	478	SER	CYS	ENGINEERED	UNP P63142
D	-18	MET	-	EXPRESSION TAG	UNP P63142
D	-17	ALA	-	EXPRESSION TAG	UNP P63142
D	-16	HIS	-	EXPRESSION TAG	UNP P63142
D	-15	HIS	-	EXPRESSION TAG	UNP P63142
D	-14	HIS	-	EXPRESSION TAG	UNP P63142
D	-13	HIS	-	EXPRESSION TAG	UNP P63142
D	-12	HIS	-	EXPRESSION TAG	UNP P63142
D	-11	HIS	-	EXPRESSION TAG	UNP P63142
D	-10	HIS	-	EXPRESSION TAG	UNP P63142
D	-9	HIS	-	EXPRESSION TAG	UNP P63142
D	-8	HIS	-	EXPRESSION TAG	UNP P63142
D	-7	HIS	-	EXPRESSION TAG	UNP P63142
D	-6	GLY	-	EXPRESSION TAG	UNP P63142
D	-5	LEU	-	EXPRESSION TAG	UNP P63142
D	-4	VAL	-	EXPRESSION TAG	UNP P63142
D	-3	PRO	-	EXPRESSION TAG	UNP P63142
D	-2	ARG	-	EXPRESSION TAG	UNP P63142
D	-1	GLY	-	EXPRESSION TAG	UNP P63142
D	0	SER	-	EXPRESSION TAG	UNP P63142
D	31	SER	CYS	ENGINEERED	UNP P63142
D	32	SER	CYS	ENGINEERED	UNP P63142
D	207	GLN	ASN	ENGINEERED	UNP P63142
D	233	TRP	PHE	ENGINEERED	UNP P63142
D	431	SER	CYS	ENGINEERED	UNP P63142
D	478	SER	CYS	ENGINEERED	UNP P63142

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is (1R)-2-{-[(S)-{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(HEXADECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: PGW) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			19	15	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C 5 5	0	0
4	B	1	Total C 5 5	0	0
4	B	1	Total C 5 5	0	0
4	B	1	Total C 8 8	0	0
4	B	1	Total C 7 7	0	0
4	B	1	Total C 7 7	0	0
4	B	1	Total C O P 20 11 8 1	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C O P 28 17 10 1	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 6 6	0	0
4	D	1	Total C O 22 17 5	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	5	Total K 5 5	0	0
5	D	5	Total K 5 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	92	Total O 92 92	0	0
6	B	46	Total O 46 46	0	0
6	C	91	Total O 91 91	0	0

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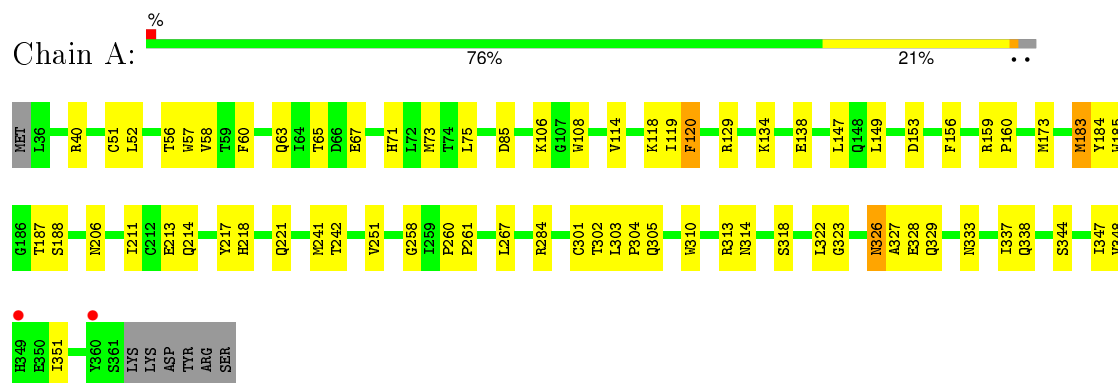
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	14	Total	O	0	0
			14	14		



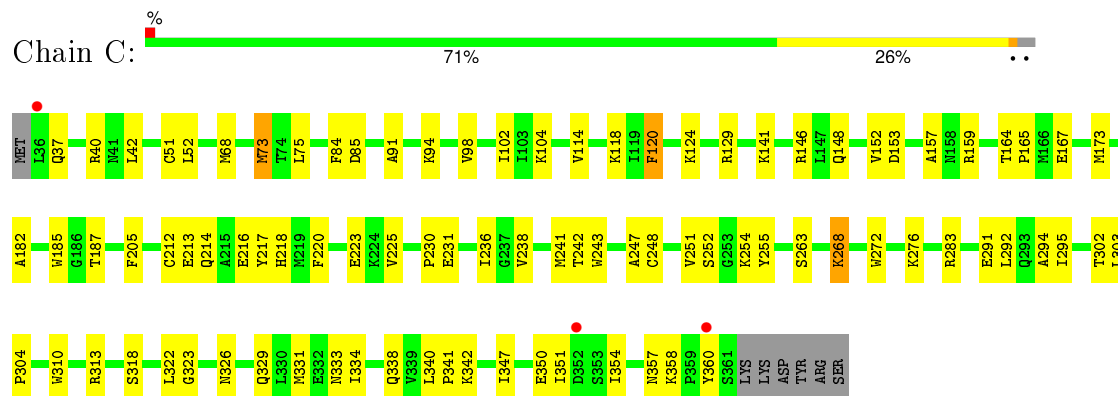
### 3 Residue-property plots

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.

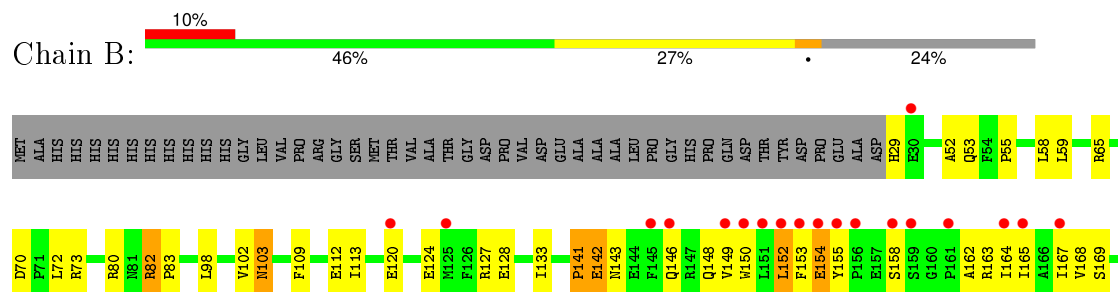
- Molecule 1: Voltage-gated potassium channel subunit beta-2

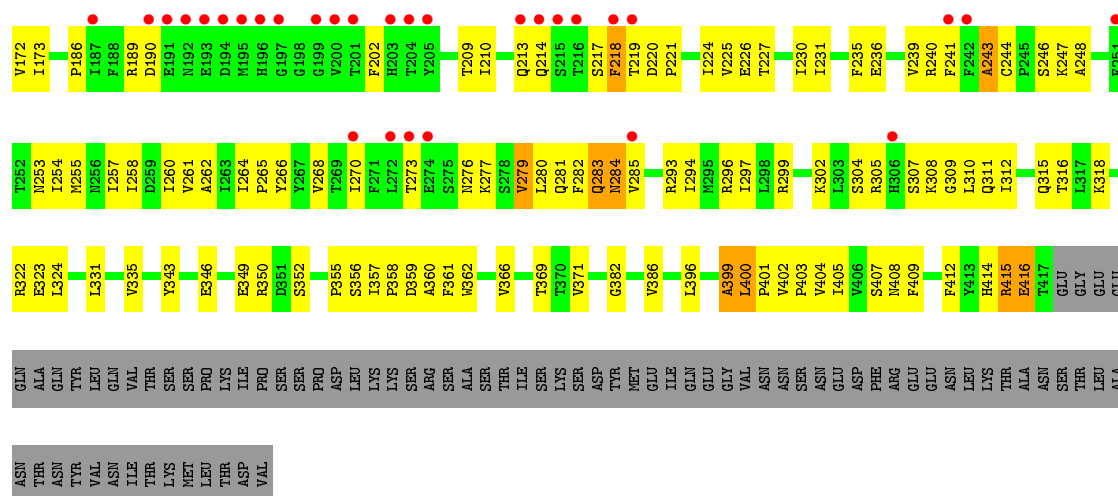


- Molecule 1: Voltage-gated potassium channel subunit beta-2

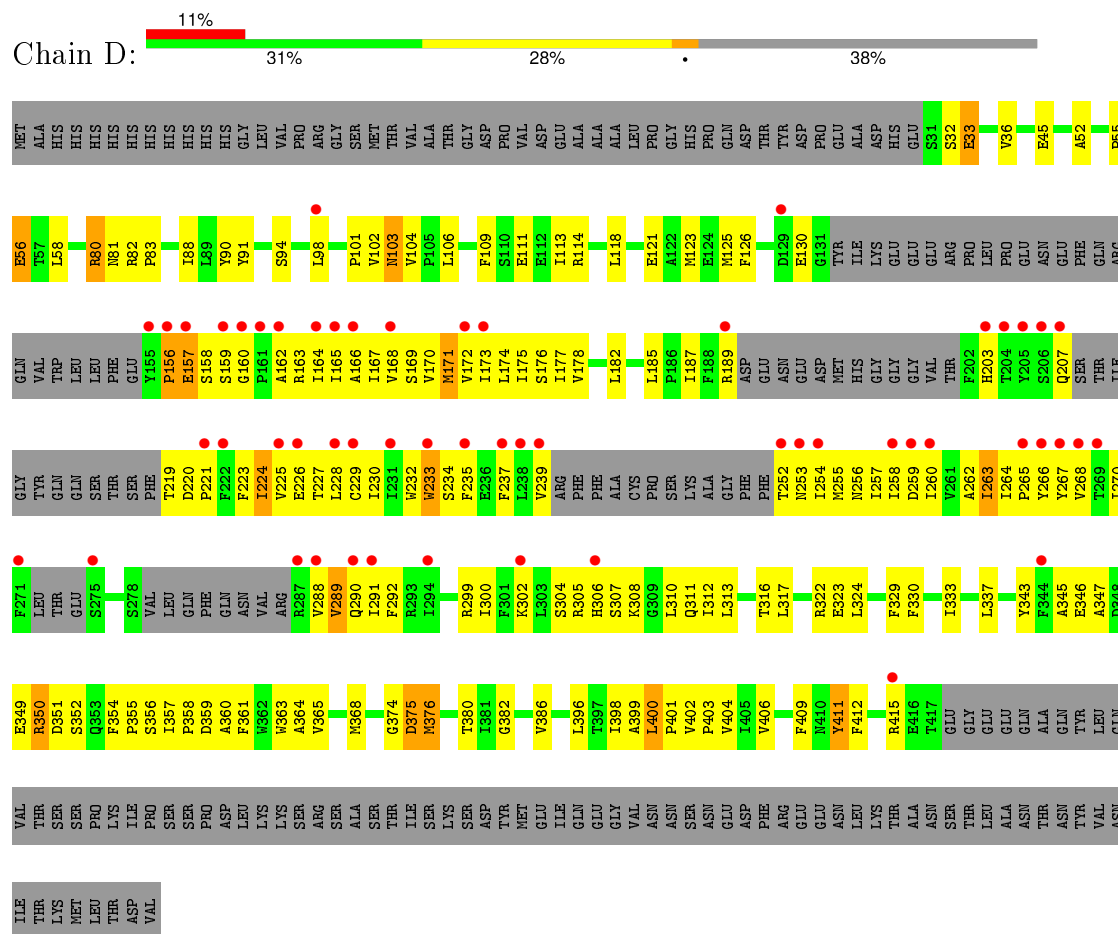


- Molecule 2: F233W mutant of the Kv2.1 paddle-Kv1.2 chimera





- Molecule 2: F233W mutant of the Kv2.1 paddle-Kv1.2 chimera



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.27Å 144.27Å 284.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 2.90 49.63 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.64-2.90) 99.6 (49.63-2.90)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.60 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.211 , 0.247 0.212 , 0.246	Depositor DCC
$R_{free}$ test set	3228 reflections (4.82%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 67.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 67125 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11308	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGW, K, NAP

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	0.42	0/2608	0.62	0/3524
1	C	0.38	0/2608	0.59	1/3524 (0.0%)
2	B	0.35	0/3199	0.54	0/4334
2	D	0.33	0/2646	0.54	0/3581
All	All	0.37	0/11061	0.57	1/14963 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	ALA	N-CA-C	-5.06	97.33	111.00

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	2556	0	2582	56	0
1	C	2556	0	2582	61	0
2	B	3116	0	3052	137	0
2	D	2584	0	2598	186	0
3	A	48	0	25	2	0
3	C	48	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	125	0	141	8	0
4	D	22	0	25	7	0
5	B	5	0	0	0	0
5	D	5	0	0	0	0
6	A	92	0	0	2	0
6	B	46	0	0	2	0
6	C	91	0	0	3	0
6	D	14	0	0	2	0
All	All	11308	0	11030	446	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 20.

All (446) 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:213:GLN:HE22	2:B:219:THR:HB	1.29	0.95
2:B:400:LEU:HB2	2:B:401:PRO:HD3	1.49	0.93
2:D:400:LEU:HB2	2:D:401:PRO:HD3	1.48	0.93
2:D:103:ASN:HD22	2:D:103:ASN:H	1.11	0.92
1:C:295:ILE:H	1:C:295:ILE:HD12	1.37	0.89
2:D:264:ILE:HB	2:D:265:PRO:HD3	1.54	0.89
1:C:333:ASN:HD21	3:C:1001:NAP:H61A	1.22	0.86
2:B:103:ASN:H	2:B:103:ASN:HD22	1.21	0.85
2:B:236:GLU:HB3	2:B:240:ARG:HH12	1.39	0.84
2:D:260:ILE:HG22	2:D:264:ILE:HD11	1.60	0.84
2:D:182:LEU:HA	2:D:185:LEU:HD13	1.59	0.83
2:B:236:GLU:HB3	2:B:240:ARG:NH1	1.94	0.82
2:B:213:GLN:HB3	2:B:220:ASP:HB2	1.60	0.82
2:D:103:ASN:H	2:D:103:ASN:ND2	1.78	0.80
2:B:152:LEU:HB2	2:B:165:ILE:HD12	1.64	0.77
2:D:267:TYR:HA	2:D:270:ILE:HD12	1.64	0.77
1:C:338:GLN:O	1:C:341:PRO:HD2	1.85	0.76
1:C:217:TYR:HB2	1:C:225:VAL:HG21	1.68	0.76
2:D:225:VAL:HG13	2:D:228:LEU:HD23	1.68	0.76
2:D:355:PRO:HB2	2:D:359:ASP:OD2	1.86	0.75
2:B:82:ARG:HB2	2:B:83:PRO:HD3	1.67	0.74
2:B:98:LEU:HD21	2:B:113:ILE:HD13	1.70	0.74
2:D:259:ASP:HB2	2:D:302:LYS:NZ	2.02	0.74
2:D:265:PRO:HA	2:D:292:PHE:HD2	1.53	0.73
2:B:186:PRO:HG3	2:B:189:ARG:NH2	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:257:ILE:HD13	2:D:260:ILE:HD12	1.71	0.72
2:B:350:ARG:HB3	2:B:350:ARG:NH1	2.05	0.72
2:D:260:ILE:O	2:D:264:ILE:HG13	1.90	0.72
2:B:244:CYS:HB3	2:B:247:LYS:HD3	1.71	0.72
2:D:264:ILE:O	2:D:268:VAL:HG23	1.90	0.71
2:B:73:ARG:HD3	6:B:2061:HOH:O	1.89	0.71
2:B:168:VAL:O	2:B:172:VAL:HG23	1.90	0.70
1:C:75:LEU:HD23	1:C:331:MET:HE3	1.72	0.70
2:D:98:LEU:HD21	2:D:113:ILE:HD13	1.72	0.70
2:B:213:GLN:NE2	2:B:219:THR:HB	2.06	0.69
1:C:326:ASN:ND2	1:C:329:GLN:HG3	2.07	0.69
1:A:333:ASN:HD21	3:A:1001:NAP:H61A	1.39	0.69
2:B:152:LEU:HB3	2:B:162:ALA:HB2	1.73	0.69
2:D:166:ALA:HB1	2:D:306:HIS:CD2	2.28	0.69
2:D:288:VAL:HG12	2:D:289:VAL:H	1.55	0.69
2:D:288:VAL:O	2:D:289:VAL:HG22	1.93	0.69
2:B:260:ILE:HG22	2:B:264:ILE:HD11	1.75	0.68
2:B:361:PHE:HB2	4:B:601:PGW:H2	1.75	0.68
1:C:295:ILE:HD12	1:C:295:ILE:N	2.08	0.68
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.74	0.68
2:B:323:GLU:CD	2:B:323:GLU:H	1.98	0.68
2:D:82:ARG:HB2	2:D:83:PRO:HD3	1.77	0.67
2:D:237:PHE:HE1	2:D:260:ILE:HG12	1.60	0.66
2:D:411:TYR:CZ	2:D:415:ARG:HD3	2.30	0.66
2:D:227:THR:HA	2:D:230:ILE:HB	1.76	0.66
2:D:230:ILE:HG21	2:D:266:TYR:CE2	2.30	0.66
2:B:315:GLN:HE21	4:B:610:PGW:H01	1.61	0.66
2:D:254:ILE:HG23	2:D:255:MET:H	1.60	0.65
2:B:109:PHE:CE2	2:B:113:ILE:HD11	2.31	0.65
2:B:244:CYS:H	2:B:247:LYS:HZ3	1.42	0.65
2:D:322:ARG:HH11	2:D:322:ARG:HG3	1.62	0.65
2:D:173:ILE:HD13	2:D:302:LYS:HB3	1.80	0.64
1:C:331:MET:HE2	1:C:334:ILE:HD12	1.79	0.64
2:D:227:THR:HA	2:D:230:ILE:CG1	2.28	0.64
2:D:109:PHE:CE2	2:D:113:ILE:HD11	2.33	0.64
2:D:343:TYR:CE1	2:D:356:SER:HA	2.33	0.64
2:D:288:VAL:HG12	2:D:289:VAL:N	2.14	0.63
2:B:164:ILE:O	2:B:168:VAL:HG23	1.99	0.63
2:B:120:GLU:O	2:B:124:GLU:HG3	1.98	0.63
2:B:396:LEU:O	2:B:400:LEU:HG	1.99	0.63
2:B:350:ARG:HH11	2:B:350:ARG:HB3	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:GLU:HB2	2:D:352:SER:HB2	1.79	0.63
1:A:326:ASN:ND2	1:A:329:GLN:H	1.97	0.62
2:D:106:LEU:HD11	2:D:130:GLU:HG2	1.80	0.62
2:B:280:LEU:HD12	2:B:280:LEU:H	1.64	0.62
2:B:282:PHE:C	2:B:284:ASN:H	2.02	0.62
2:D:81:ASN:HA	6:D:2057:HOH:O	1.99	0.62
1:A:326:ASN:HD22	1:A:328:GLU:N	1.97	0.62
1:C:295:ILE:H	1:C:295:ILE:CD1	2.10	0.61
2:B:240:ARG:HG3	2:B:240:ARG:HH11	1.65	0.61
2:D:121:GLU:O	2:D:125:MET:HG2	2.01	0.61
2:B:210:ILE:HD11	2:B:273:THR:HG21	1.83	0.61
2:D:90:TYR:CE2	2:D:94:SER:HB3	2.36	0.60
1:C:167:GLU:HG3	1:C:205:PHE:CE1	2.37	0.60
1:A:40:ARG:HD2	1:A:318:SER:O	2.01	0.60
2:D:357:ILE:HB	2:D:358:PRO:HD3	1.83	0.60
2:B:331:LEU:O	2:B:335:VAL:HG23	2.01	0.60
2:D:402:VAL:HB	2:D:403:PRO:HD3	1.84	0.60
2:B:213:GLN:HB3	2:B:220:ASP:CB	2.32	0.59
1:C:141:LYS:HD2	6:C:2091:HOH:O	2.00	0.59
2:B:276:ASN:HB3	2:B:281:GLN:HB3	1.85	0.59
1:A:326:ASN:HD21	1:A:328:GLU:HB2	1.67	0.59
2:D:235:PHE:O	2:D:239:VAL:HG23	2.03	0.59
2:D:364:ALA:O	2:D:368:MET:HG3	2.02	0.59
2:B:262:ALA:CB	2:B:302:LYS:HD2	2.32	0.59
1:C:292:LEU:HA	1:C:295:ILE:HD13	1.85	0.59
2:B:103:ASN:H	2:B:103:ASN:ND2	1.97	0.59
2:D:185:LEU:O	2:D:189:ARG:HG2	2.03	0.59
2:D:375:ASP:O	2:D:376:MET:HB2	2.01	0.58
2:D:52:ALA:O	2:D:55:PRO:HD3	2.03	0.58
2:D:172:VAL:HG12	2:D:172:VAL:O	2.02	0.58
2:D:227:THR:HA	2:D:230:ILE:CB	2.33	0.58
2:D:162:ALA:HA	2:D:165:ILE:CD1	2.32	0.58
1:C:236:ILE:HG13	1:C:238:VAL:HG23	1.85	0.58
2:D:254:ILE:HG23	2:D:255:MET:N	2.18	0.58
2:B:361:PHE:CB	4:B:601:PGW:H2	2.33	0.58
4:B:608:PGW:O02	4:B:608:PGW:O11	2.22	0.58
2:D:221:PRO:C	2:D:223:PHE:H	2.06	0.57
2:D:255:MET:HG3	2:D:305:ARG:NH2	2.18	0.57
2:D:288:VAL:C	2:D:290:GLN:H	2.06	0.57
1:A:326:ASN:HD21	1:A:329:GLN:H	1.52	0.57
2:B:264:ILE:O	2:B:268:VAL:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:259:ASP:HB2	2:D:302:LYS:HZ3	1.66	0.57
1:A:258:GLY:O	1:A:260:PRO:HD3	2.05	0.57
2:D:396:LEU:O	2:D:400:LEU:HG	2.05	0.57
2:D:253:ASN:HB3	2:D:256:ASN:ND2	2.19	0.57
2:B:244:CYS:H	2:B:247:LYS:NZ	2.03	0.57
2:D:113:ILE:HG23	2:D:118:LEU:HD12	1.87	0.57
2:D:267:TYR:HA	2:D:270:ILE:CD1	2.34	0.57
4:B:601:PGW:O02	4:B:601:PGW:H01	2.03	0.57
2:D:365:VAL:HG21	4:D:601:PGW:H6A	1.87	0.57
2:D:160:GLY:O	2:D:164:ILE:HG12	2.05	0.57
2:D:109:PHE:O	2:D:113:ILE:HG13	2.05	0.56
4:D:601:PGW:O02	4:D:601:PGW:H01	2.04	0.56
2:B:382:GLY:O	2:B:386:VAL:HG23	2.06	0.56
2:B:294:ILE:O	2:B:297:ILE:HG22	2.06	0.56
2:D:56:GLU:CD	2:D:56:GLU:H	2.08	0.56
1:A:159:ARG:HA	1:A:188:SER:O	2.06	0.56
1:C:326:ASN:HD21	1:C:329:GLN:HG3	1.70	0.56
2:D:32:SER:O	2:D:33:GLU:C	2.44	0.55
2:D:58:LEU:HD23	2:D:58:LEU:C	2.26	0.55
2:D:173:ILE:C	2:D:175:ILE:H	2.08	0.55
2:B:281:GLN:O	2:B:284:ASN:HB3	2.07	0.55
2:D:350:ARG:HD2	2:D:350:ARG:O	2.07	0.55
2:D:165:ILE:O	2:D:168:VAL:HG12	2.07	0.54
2:D:402:VAL:O	2:D:406:VAL:HG23	2.06	0.54
2:B:309:GLY:HA2	2:B:312:ILE:HD12	1.87	0.54
2:D:103:ASN:N	2:D:103:ASN:HD22	1.93	0.54
2:D:156:PRO:O	2:D:158:SER:N	2.35	0.54
2:D:227:THR:OG1	2:D:230:ILE:HD12	2.07	0.54
1:C:340:LEU:HB3	1:C:341:PRO:HD3	1.88	0.54
2:D:171:MET:SD	2:D:171:MET:N	2.80	0.54
1:A:302:THR:OG1	1:A:305:GLN:HG3	2.08	0.54
2:D:266:TYR:O	2:D:270:ILE:HG13	2.08	0.54
1:A:326:ASN:ND2	1:A:328:GLU:HB2	2.23	0.53
1:A:147:LEU:HB3	1:A:149:LEU:HD12	1.89	0.53
1:C:347:ILE:O	1:C:351:ILE:HG13	2.09	0.53
1:C:247:ALA:O	1:C:248:CYS:HB2	2.08	0.53
2:D:237:PHE:CE1	2:D:260:ILE:HG12	2.43	0.53
2:D:227:THR:C	2:D:229:CYS:H	2.11	0.53
2:D:227:THR:C	2:D:229:CYS:N	2.62	0.53
2:B:255:MET:HB3	2:B:305:ARG:NH2	2.23	0.53
2:D:350:ARG:HG3	2:D:350:ARG:HH11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:ARG:HH11	2:D:114:ARG:HG3	1.74	0.53
2:D:203:HIS:O	2:D:207:GLN:HB3	2.08	0.53
2:B:103:ASN:HD22	2:B:103:ASN:N	2.00	0.53
2:D:346:GLU:OE2	2:D:380:THR:HG23	2.09	0.53
2:B:241:PHE:O	2:B:247:LYS:NZ	2.39	0.53
1:C:187:THR:O	1:C:213:GLU:HA	2.09	0.53
2:D:308:LYS:O	2:D:312:ILE:HG13	2.09	0.53
2:D:178:VAL:O	2:D:182:LEU:HG	2.08	0.52
2:D:189:ARG:HH11	2:D:189:ARG:HG3	1.74	0.52
2:B:163:ARG:O	2:B:167:ILE:HG12	2.09	0.52
1:A:251:VAL:HG12	1:A:251:VAL:O	2.08	0.52
1:A:326:ASN:HD22	1:A:328:GLU:H	1.57	0.52
1:C:152:VAL:O	1:C:182:ALA:HA	2.08	0.52
1:C:350:GLU:O	1:C:354:ILE:HG13	2.10	0.52
1:C:214:GLN:HA	1:C:241:MET:O	2.09	0.52
2:D:313:LEU:O	2:D:317:LEU:HG	2.09	0.52
1:A:71:HIS:CD2	1:A:327:ALA:HB2	2.45	0.52
1:C:218:HIS:CE1	1:C:220:PHE:HB2	2.45	0.52
2:B:277:LYS:HE3	6:B:2123:HOH:O	2.10	0.52
2:B:262:ALA:HB1	2:B:302:LYS:HD2	1.90	0.52
2:D:349:GLU:HB3	2:D:352:SER:H	1.75	0.52
2:D:171:MET:C	2:D:173:ILE:H	2.13	0.52
2:D:259:ASP:HA	2:D:262:ALA:HB3	1.92	0.52
2:B:311:GLN:O	2:B:315:GLN:HG3	2.10	0.52
2:D:361:PHE:HD2	4:D:601:PGW:H20A	1.75	0.52
1:A:303:LEU:HB3	1:A:304:PRO:HD3	1.92	0.52
1:C:120:PHE:O	1:C:129:ARG:HA	2.10	0.51
2:B:415:ARG:HH11	2:B:415:ARG:HG2	1.76	0.51
2:B:414:HIS:C	2:B:416:GLU:H	2.14	0.51
1:C:120:PHE:CE2	1:C:159:ARG:HD3	2.46	0.51
1:C:104:LYS:NZ	1:C:148:GLN:HE22	2.07	0.51
2:D:374:GLY:C	2:D:376:MET:H	2.13	0.51
1:A:120:PHE:O	1:A:129:ARG:HA	2.10	0.51
2:B:53:GLN:C	2:B:55:PRO:HD3	2.31	0.51
1:C:114:VAL:HA	1:C:153:ASP:OD2	2.10	0.51
2:D:316:THR:HG21	2:D:409:PHE:HB2	1.92	0.51
2:B:324:LEU:HD13	2:B:405:ILE:HD13	1.93	0.51
2:B:414:HIS:O	2:B:416:GLU:N	2.37	0.51
2:B:280:LEU:N	2:B:280:LEU:HD12	2.26	0.50
2:D:88:ILE:O	2:D:91:TYR:HB3	2.11	0.50
1:C:310:TRP:O	1:C:313:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:400:LEU:O	2:D:403:PRO:HD2	2.11	0.50
2:D:258:ILE:CG2	2:D:302:LYS:HA	2.41	0.50
1:A:326:ASN:ND2	1:A:328:GLU:N	2.59	0.50
2:D:221:PRO:HA	2:D:224:ILE:HB	1.93	0.50
2:D:329:PHE:O	2:D:333:ILE:HG12	2.12	0.50
2:D:400:LEU:HB2	2:D:401:PRO:CD	2.32	0.50
2:D:259:ASP:O	2:D:263:ILE:HG12	2.12	0.50
2:B:243:ALA:N	2:B:247:LYS:HZ1	2.10	0.50
2:D:162:ALA:HA	2:D:165:ILE:HD12	1.93	0.50
2:D:169:SER:O	2:D:173:ILE:HG13	2.12	0.50
2:B:357:ILE:HB	2:B:358:PRO:HD3	1.94	0.50
2:D:177:ILE:HD11	2:D:300:ILE:HG13	1.94	0.50
2:D:304:SER:HA	2:D:310:LEU:HD23	1.92	0.50
2:B:102:VAL:HG23	2:B:103:ASN:N	2.27	0.50
1:C:73:MET:HE3	1:C:84:PHE:CD2	2.47	0.50
2:D:354:PHE:HE1	2:D:376:MET:HE2	1.77	0.49
2:B:362:TRP:O	2:B:366:VAL:HG23	2.12	0.49
2:B:29:HIS:HB2	2:B:52:ALA:HB3	1.93	0.49
2:D:260:ILE:HG22	2:D:264:ILE:CD1	2.37	0.49
2:B:318:LYS:HD2	4:B:610:PGW:H22	1.94	0.49
2:D:253:ASN:O	2:D:257:ILE:HG12	2.12	0.49
1:A:313:ARG:HG2	1:A:313:ARG:HH11	1.76	0.49
2:D:123:MET:O	2:D:126:PHE:HB3	2.11	0.49
2:B:169:SER:O	2:B:173:ILE:HG13	2.12	0.49
1:C:302:THR:OG1	1:C:304:PRO:HD2	2.13	0.49
2:B:343:TYR:CE1	2:B:356:SER:HA	2.48	0.49
1:C:333:ASN:ND2	3:C:1001:NAP:H61A	2.02	0.49
2:B:261:VAL:HA	2:B:264:ILE:HD12	1.95	0.49
2:B:282:PHE:C	2:B:284:ASN:N	2.66	0.49
2:D:308:LYS:HA	2:D:311:GLN:CG	2.43	0.49
2:D:361:PHE:CD2	4:D:601:PGW:H20A	2.48	0.49
1:A:52:LEU:HD13	1:A:322:LEU:HD11	1.93	0.49
2:B:240:ARG:HG3	2:B:240:ARG:NH1	2.27	0.49
1:A:338:GLN:CD	1:A:338:GLN:N	2.65	0.49
2:B:141:PRO:O	2:B:143:ASN:N	2.46	0.49
2:B:53:GLN:O	2:B:55:PRO:HD3	2.13	0.49
2:B:296:ARG:HE	2:B:299:ARG:NH2	2.11	0.49
1:C:268:LYS:HB3	1:C:268:LYS:NZ	2.28	0.49
1:A:118:LYS:CG	1:A:156:PHE:HB2	2.43	0.48
2:B:221:PRO:O	2:B:225:VAL:HG23	2.12	0.48
1:C:120:PHE:CD1	1:C:159:ARG:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:THR:HG22	1:A:60:PHE:CD1	2.48	0.48
2:D:403:PRO:O	2:D:406:VAL:HB	2.12	0.48
1:C:295:ILE:HD11	1:C:354:ILE:HD11	1.94	0.48
2:B:243:ALA:H	2:B:247:LYS:NZ	2.11	0.48
2:B:227:THR:O	2:B:231:ILE:HG12	2.12	0.48
2:D:227:THR:HA	2:D:230:ILE:HG13	1.95	0.48
1:A:120:PHE:CD1	1:A:159:ARG:HG3	2.48	0.48
2:B:355:PRO:HG2	2:B:359:ASP:OD2	2.13	0.48
2:D:187:ILE:O	2:D:187:ILE:HG22	2.13	0.48
2:B:322:ARG:HH11	2:B:322:ARG:HG3	1.79	0.48
1:A:323:GLY:HA3	3:A:1001:NAP:H51A	1.95	0.48
2:B:308:LYS:O	2:B:312:ILE:HG13	2.14	0.48
2:B:230:ILE:HG12	2:B:266:TYR:CG	2.49	0.48
1:C:40:ARG:HD2	1:C:51:CYS:HB3	1.95	0.48
1:C:52:LEU:HD13	1:C:322:LEU:HD11	1.96	0.48
1:A:57:TRP:CD2	1:A:58:VAL:HG23	2.48	0.48
2:D:233:TRP:HA	2:D:233:TRP:CE3	2.48	0.47
1:C:323:GLY:HA3	3:C:1001:NAP:H51A	1.96	0.47
1:C:333:ASN:N	1:C:333:ASN:HD22	2.11	0.47
2:D:350:ARG:HG3	2:D:350:ARG:NH1	2.28	0.47
1:A:310:TRP:O	1:A:313:ARG:HG2	2.14	0.47
2:D:337:LEU:C	2:D:337:LEU:HD23	2.34	0.47
2:B:29:HIS:HB2	2:B:52:ALA:CB	2.44	0.47
1:C:42:LEU:HD11	1:C:212:CYS:SG	2.54	0.47
2:D:288:VAL:O	2:D:290:GLN:N	2.47	0.47
2:B:282:PHE:HA	2:B:285:VAL:HG12	1.96	0.47
1:C:40:ARG:HD3	1:C:318:SER:O	2.14	0.47
2:D:264:ILE:HB	2:D:265:PRO:CD	2.37	0.47
2:D:175:ILE:HA	2:D:178:VAL:CG2	2.45	0.47
1:C:291:GLU:O	1:C:294:ALA:HB3	2.14	0.47
2:D:322:ARG:NH1	2:D:322:ARG:HG3	2.28	0.47
1:C:272:TRP:O	1:C:276:LYS:HG2	2.15	0.47
4:B:606:PGW:H3	4:B:609:PGW:H17	1.96	0.47
1:A:187:THR:O	1:A:213:GLU:HA	2.14	0.47
1:C:85:ASP:OD1	1:C:118:LYS:NZ	2.48	0.47
2:D:80:ARG:HG2	6:D:2061:HOH:O	2.15	0.47
1:C:292:LEU:HD21	1:C:351:ILE:HG23	1.96	0.47
2:B:189:ARG:HG3	2:B:189:ARG:HH11	1.80	0.47
2:B:399:ALA:O	2:B:403:PRO:HD3	2.14	0.47
2:D:171:MET:HB3	2:D:175:ILE:HD12	1.95	0.47
1:C:217:TYR:HB3	1:C:242:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:PRO:C	2:D:158:SER:H	2.17	0.46
2:D:351:ASP:O	2:D:352:SER:C	2.53	0.46
2:D:361:PHE:CB	4:D:601:PGW:H2	2.45	0.46
2:B:346:GLU:O	2:B:349:GLU:HB2	2.15	0.46
2:D:182:LEU:O	2:D:185:LEU:HB2	2.16	0.46
2:D:266:TYR:HD2	2:D:267:TYR:CE1	2.34	0.46
2:D:98:LEU:HD23	2:D:126:PHE:HB2	1.98	0.46
2:B:264:ILE:HB	2:B:265:PRO:HD3	1.96	0.46
2:D:157:GLU:HA	2:D:163:ARG:CG	2.46	0.46
1:C:303:LEU:HB3	1:C:304:PRO:HD3	1.97	0.46
2:D:111:GLU:O	2:D:114:ARG:HB3	2.16	0.46
2:B:226:GLU:O	2:B:230:ILE:HD13	2.16	0.46
2:B:214:GLN:NE2	2:B:270:ILE:HG12	2.30	0.46
2:B:408:ASN:O	2:B:412:PHE:HD2	1.99	0.46
2:B:153:PHE:CE2	2:B:239:VAL:HG11	2.51	0.46
2:D:343:TYR:C	2:D:345:ALA:H	2.20	0.46
1:C:91:ALA:O	1:C:94:LYS:HB2	2.16	0.46
2:D:291:ILE:HG22	2:D:291:ILE:O	2.15	0.46
2:B:149:VAL:O	2:B:152:LEU:HD12	2.16	0.46
2:D:101:PRO:HB2	2:D:104:VAL:HG23	1.98	0.46
1:C:146:ARG:HD3	6:C:2049:HOH:O	2.15	0.46
2:D:266:TYR:CZ	2:D:270:ILE:HD11	2.51	0.45
2:B:186:PRO:O	2:B:190:ASP:HB2	2.16	0.45
2:B:109:PHE:O	2:B:113:ILE:HG13	2.15	0.45
1:A:183:MET:HB3	1:A:184:TYR:CD1	2.52	0.45
2:D:258:ILE:O	2:D:302:LYS:HD3	2.17	0.45
2:B:360:ALA:O	2:B:361:PHE:C	2.55	0.45
2:D:363:TRP:HB2	2:D:376:MET:HE2	1.97	0.45
2:D:308:LYS:HA	2:D:311:GLN:HG2	1.98	0.45
2:B:82:ARG:HB2	2:B:83:PRO:CD	2.44	0.45
1:C:68:MET:HA	1:C:68:MET:HE2	1.97	0.45
1:C:173:MET:HG3	1:C:185:TRP:CE3	2.51	0.45
1:C:98:VAL:O	1:C:102:ILE:HG13	2.17	0.45
2:D:176:SER:OG	2:D:299:ARG:NH1	2.49	0.45
1:C:252:SER:OG	1:C:254:LYS:HG2	2.16	0.45
2:D:230:ILE:HG21	2:D:266:TYR:CD2	2.51	0.45
2:B:369:THR:OG1	2:B:371:VAL:HG23	2.17	0.45
2:B:202:PHE:HB2	2:B:279:VAL:CG2	2.47	0.45
2:D:354:PHE:CE1	2:D:376:MET:HE2	2.52	0.45
2:B:246:SER:C	2:B:248:ALA:H	2.19	0.45
2:B:235:PHE:O	2:B:239:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:229:CYS:HA	2:D:232:TRP:CB	2.47	0.45
2:B:226:GLU:OE1	2:B:296:ARG:NH2	2.49	0.45
1:A:326:ASN:HD22	1:A:326:ASN:C	2.20	0.44
2:D:324:LEU:H	2:D:324:LEU:HD22	1.83	0.44
2:B:400:LEU:CB	2:B:401:PRO:HD3	2.33	0.44
2:B:307:SER:O	2:B:311:GLN:HG3	2.17	0.44
2:D:106:LEU:CD1	2:D:130:GLU:HG2	2.45	0.44
4:B:608:PGW:H02	4:B:608:PGW:O12	2.17	0.44
1:C:251:VAL:O	1:C:251:VAL:HG12	2.17	0.44
2:B:146:GLN:C	2:B:148:GLN:H	2.21	0.44
1:A:344:SER:O	1:A:348:VAL:HG23	2.18	0.44
1:A:71:HIS:HD2	1:A:327:ALA:HB2	1.81	0.44
2:D:167:ILE:HA	2:D:170:VAL:HG23	1.99	0.44
1:A:314:ASN:HB2	6:A:2035:HOH:O	2.18	0.44
1:A:217:TYR:HB3	1:A:242:THR:HB	1.99	0.44
2:B:400:LEU:HB2	2:B:401:PRO:CD	2.34	0.44
2:D:219:THR:O	2:D:220:ASP:HB2	2.17	0.44
2:D:304:SER:CA	2:D:310:LEU:HD23	2.48	0.44
2:D:172:VAL:HG12	2:D:233:TRP:CZ2	2.53	0.44
2:D:330:PHE:O	2:D:333:ILE:HB	2.17	0.44
2:B:70:ASP:OD1	2:B:70:ASP:C	2.55	0.44
2:D:302:LYS:HA	2:D:302:LYS:HD2	1.82	0.43
2:D:220:ASP:O	2:D:224:ILE:HG13	2.17	0.43
2:B:243:ALA:N	2:B:247:LYS:NZ	2.65	0.43
2:D:109:PHE:HE2	2:D:113:ILE:HD11	1.79	0.43
1:A:260:PRO:HA	1:A:261:PRO:HD3	1.90	0.43
2:B:141:PRO:O	2:B:142:GLU:C	2.57	0.43
1:A:301:CYS:HB2	1:A:305:GLN:OE1	2.18	0.43
2:B:253:ASN:OD1	2:B:255:MET:HB2	2.18	0.43
1:C:104:LYS:HZ2	1:C:148:GLN:HE22	1.66	0.43
2:D:102:VAL:HG23	2:D:103:ASN:N	2.33	0.43
2:D:264:ILE:CB	2:D:265:PRO:HD3	2.35	0.43
2:D:233:TRP:HE3	2:D:233:TRP:HA	1.84	0.43
2:D:176:SER:OG	2:D:299:ARG:HD3	2.18	0.43
2:B:59:LEU:O	2:B:65:ARG:NH1	2.49	0.43
2:D:173:ILE:C	2:D:175:ILE:N	2.72	0.43
1:A:67:GLU:H	1:A:67:GLU:CD	2.22	0.43
2:D:165:ILE:HG22	2:D:165:ILE:O	2.18	0.43
2:D:225:VAL:HG13	2:D:228:LEU:CD2	2.45	0.43
2:D:346:GLU:O	2:D:347:ALA:C	2.57	0.43
2:D:258:ILE:O	2:D:258:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:VAL:O	2:B:285:VAL:HG22	2.18	0.43
1:A:347:ILE:O	1:A:351:ILE:HG13	2.19	0.43
2:D:400:LEU:CB	2:D:401:PRO:HD3	2.32	0.43
2:B:316:THR:HG21	2:B:409:PHE:HB2	2.00	0.43
1:A:326:ASN:C	1:A:326:ASN:ND2	2.72	0.43
1:A:159:ARG:HB2	1:A:160:PRO:HD2	2.00	0.43
1:A:106:LYS:HG3	1:A:108:TRP:CH2	2.54	0.43
2:D:221:PRO:HA	2:D:224:ILE:HD12	1.99	0.43
2:D:288:VAL:C	2:D:290:GLN:N	2.70	0.43
2:D:114:ARG:NH1	2:D:114:ARG:HG3	2.34	0.43
2:B:254:ILE:O	2:B:258:ILE:HG13	2.19	0.43
2:B:127:ARG:HG2	2:B:127:ARG:HH11	1.84	0.43
1:A:134:LYS:O	1:A:138:GLU:HG3	2.19	0.43
2:D:175:ILE:HA	2:D:178:VAL:HG23	2.01	0.42
2:B:58:LEU:C	2:B:58:LEU:HD23	2.39	0.42
1:A:63:GLN:NE2	1:A:267:LEU:HD11	2.35	0.42
2:B:150:TRP:HE1	2:B:155:TYR:HE2	1.66	0.42
2:D:164:ILE:HG22	2:D:164:ILE:O	2.18	0.42
1:A:119:ILE:O	1:A:120:PHE:HB2	2.19	0.42
2:B:343:TYR:HE1	2:B:356:SER:HA	1.83	0.42
1:A:114:VAL:HA	1:A:153:ASP:OD2	2.19	0.42
2:B:217:SER:O	2:B:218:PHE:C	2.58	0.42
2:D:382:GLY:O	2:D:386:VAL:HG23	2.20	0.42
2:B:404:VAL:O	2:B:407:SER:HB3	2.19	0.42
2:B:349:GLU:HB2	2:B:352:SER:HB2	2.01	0.42
2:B:127:ARG:HG2	2:B:127:ARG:NH1	2.35	0.42
2:D:168:VAL:O	2:D:168:VAL:HG22	2.20	0.42
2:D:361:PHE:HB2	4:D:601:PGW:H2	2.02	0.42
2:B:255:MET:CE	2:B:305:ARG:HB2	2.50	0.42
2:B:402:VAL:HB	2:B:403:PRO:HD3	2.00	0.42
2:B:246:SER:C	2:B:248:ALA:N	2.73	0.42
1:A:51:CYS:SG	1:A:337:ILE:HD11	2.59	0.42
2:B:209:THR:O	2:B:293:ARG:HD2	2.19	0.42
2:B:304:SER:CA	2:B:310:LEU:HD23	2.50	0.42
2:D:171:MET:O	2:D:175:ILE:HB	2.18	0.42
1:A:65:THR:HB	1:A:67:GLU:OE1	2.19	0.42
2:B:218:PHE:HB3	2:B:224:ILE:HG12	2.00	0.42
1:C:216:GLU:HB2	1:C:243:TRP:CZ2	2.55	0.42
2:D:323:GLU:OE1	2:D:404:VAL:HG11	2.20	0.42
1:C:357:ASN:O	1:C:358:LYS:C	2.58	0.42
1:A:284:ARG:HB2	1:A:284:ARG:NH1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LYS:HG3	6:C:2082:HOH:O	2.19	0.42
2:B:153:PHE:O	2:B:154:GLU:HB2	2.20	0.42
2:D:307:SER:O	2:D:311:GLN:HG2	2.20	0.42
2:D:225:VAL:O	2:D:225:VAL:HG12	2.20	0.42
2:B:277:LYS:O	2:B:277:LYS:HG3	2.20	0.42
2:B:230:ILE:HG21	2:B:266:TYR:CD2	2.55	0.42
1:A:173:MET:HG3	1:A:185:TRP:CE3	2.55	0.42
1:A:218:HIS:CE1	1:A:221:GLN:HB2	2.55	0.42
1:C:331:MET:CE	1:C:334:ILE:HD12	2.48	0.41
2:D:252:THR:HG22	2:D:253:ASN:N	2.35	0.41
1:A:85:ASP:OD1	1:A:118:LYS:NZ	2.49	0.41
2:B:72:LEU:HA	2:B:72:LEU:HD23	1.89	0.41
1:A:337:ILE:HA	1:A:337:ILE:HD13	1.87	0.41
1:C:255:TYR:OH	1:C:263:SER:HB2	2.20	0.41
2:D:171:MET:C	2:D:173:ILE:N	2.72	0.41
2:D:166:ALA:HB1	2:D:306:HIS:HD2	1.84	0.41
2:D:160:GLY:CA	2:D:163:ARG:HB3	2.50	0.41
2:B:80:ARG:NH1	2:B:112:GLU:OE2	2.53	0.41
2:D:36:VAL:HG22	2:D:45:GLU:HG2	2.01	0.41
2:D:258:ILE:HG22	2:D:302:LYS:HA	2.02	0.41
2:B:244:CYS:N	2:B:247:LYS:NZ	2.68	0.41
2:B:399:ALA:O	2:B:403:PRO:CD	2.69	0.41
1:C:164:THR:HA	1:C:165:PRO:HD3	1.93	0.41
2:D:258:ILE:HG21	2:D:302:LYS:HA	2.01	0.41
2:B:323:GLU:N	2:B:323:GLU:CD	2.72	0.41
4:D:601:PGW:O02	4:D:601:PGW:H03A	2.20	0.41
2:B:304:SER:HA	2:B:310:LEU:HD23	2.01	0.41
2:D:398:ILE:O	2:D:402:VAL:HG23	2.21	0.41
2:D:234:SER:HA	2:D:237:PHE:HB3	2.01	0.41
2:D:262:ALA:O	2:D:263:ILE:HG23	2.20	0.41
2:D:226:GLU:HG3	2:D:230:ILE:HD11	2.03	0.41
1:C:225:VAL:O	1:C:230:PRO:HD3	2.21	0.41
2:D:288:VAL:CG1	2:D:289:VAL:H	2.28	0.41
2:B:257:ILE:O	2:B:261:VAL:HG23	2.21	0.41
2:B:282:PHE:O	2:B:284:ASN:N	2.54	0.41
2:D:160:GLY:O	2:D:163:ARG:HB3	2.20	0.41
2:D:229:CYS:HA	2:D:232:TRP:HB2	2.03	0.41
2:B:414:HIS:C	2:B:416:GLU:N	2.74	0.41
2:D:173:ILE:HG12	2:D:233:TRP:HZ2	1.86	0.40
2:D:225:VAL:O	2:D:228:LEU:HB3	2.21	0.40
2:D:360:ALA:O	2:D:361:PHE:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:THR:OG1	1:A:304:PRO:HD2	2.21	0.40
1:C:313:ARG:HG2	1:C:313:ARG:HH11	1.86	0.40
2:B:357:ILE:N	2:B:358:PRO:CD	2.84	0.40
1:A:214:GLN:HA	1:A:241:MET:O	2.21	0.40
2:B:210:ILE:HD11	2:B:273:THR:CG2	2.51	0.40
2:B:264:ILE:N	2:B:265:PRO:CD	2.85	0.40
2:D:255:MET:HG3	2:D:305:ARG:CZ	2.52	0.40
1:A:313:ARG:NH1	1:A:313:ARG:HG2	2.37	0.40
1:A:211:ILE:HG23	6:A:2003:HOH:O	2.20	0.40
2:D:224:ILE:HG22	2:D:225:VAL:N	2.36	0.40
2:D:288:VAL:CG1	2:D:289:VAL:N	2.83	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	324/333 (97%)	305 (94%)	18 (6%)	1 (0%)	46	79
1	C	324/333 (97%)	307 (95%)	14 (4%)	3 (1%)	21	57
2	B	387/514 (75%)	321 (83%)	52 (13%)	14 (4%)	4	18
2	D	304/514 (59%)	238 (78%)	52 (17%)	14 (5%)	3	11
All	All	1339/1694 (79%)	1171 (88%)	136 (10%)	32 (2%)	7	29

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	133	ILE
2	B	141	PRO
2	B	142	GLU
2	B	154	GLU

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Mol	Chain	Res	Type
2	D	157	GLU
2	D	289	VAL
1	A	120	PHE
2	B	158	SER
1	C	120	PHE
1	C	223	GLU
2	D	156	PRO
2	D	376	MET
2	B	243	ALA
2	B	283	GLN
2	B	399	ALA
2	D	159	SER
2	D	399	ALA
2	D	400	LEU
2	D	412	PHE
2	B	218	PHE
2	D	33	GLU
2	D	174	LEU
2	D	263	ILE
2	D	375	ASP
2	D	411	TYR
2	B	128	GLU
2	B	400	LEU
2	B	415	ARG
2	B	416	GLU
1	C	342	LYS
2	B	279	VAL
2	D	224	ILE

### 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	273/280 (98%)	268 (98%)	5 (2%)	66	90
1	C	273/280 (98%)	267 (98%)	6 (2%)	60	88
2	B	335/459 (73%)	330 (98%)	5 (2%)	72	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	284/459 (62%)	278 (98%)	6 (2%)	61 88
All	All	1165/1478 (79%)	1143 (98%)	22 (2%)	65 89

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	MET
1	A	75	LEU
1	A	183	MET
1	A	206	ASN
1	A	326	ASN
2	B	82	ARG
2	B	103	ASN
2	B	152	LEU
2	B	283	GLN
2	B	284	ASN
1	C	37	GLN
1	C	73	MET
1	C	231	GLU
1	C	268	LYS
1	C	283	ARG
1	C	360	TYR
2	D	56	GLU
2	D	80	ARG
2	D	103	ASN
2	D	171	MET
2	D	233	TRP
2	D	350	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	71	HIS
1	A	148	GLN
1	A	204	GLN
1	A	286	GLN
1	A	314	ASN
1	A	326	ASN
1	A	333	ASN
2	B	53	GLN

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Mol	Chain	Res	Type
2	B	103	ASN
2	B	213	GLN
2	B	214	GLN
2	B	315	GLN
1	C	37	GLN
1	C	71	HIS
1	C	148	GLN
1	C	163	ASN
1	C	204	GLN
1	C	333	ASN
2	D	47	GLN
2	D	53	GLN
2	D	103	ASN
2	D	256	ASN
2	D	311	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 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 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	NAP	A	1001	-	42,52,52	1.23	5 (11%)	54,80,80	1.24	5 (9%)
4	PGW	B	601	-	18,18,50	0.59	0	19,19,56	1.28	3 (15%)
4	PGW	B	602	-	4,4,50	0.35	0	3,3,56	0.40	0
4	PGW	B	603	-	4,4,50	0.35	0	3,3,56	0.40	0
4	PGW	B	604	-	4,4,50	0.35	0	3,3,56	0.40	0
4	PGW	B	605	-	7,7,50	0.34	0	6,6,56	0.51	0
4	PGW	B	606	-	6,6,50	0.34	0	5,5,56	0.47	0
4	PGW	B	607	-	6,6,50	0.35	0	5,5,56	0.46	0
4	PGW	B	608	-	19,19,50	0.86	0	22,24,56	1.31	4 (18%)
4	PGW	B	609	-	5,5,50	0.34	0	4,4,56	0.39	0
4	PGW	B	610	-	27,27,50	0.75	1 (3%)	27,32,56	1.39	3 (11%)
4	PGW	B	611	-	8,8,50	0.34	0	7,7,56	0.50	0
4	PGW	B	612	-	5,5,50	0.35	0	4,4,56	0.38	0
3	NAP	C	1001	-	42,52,52	1.26	5 (11%)	54,80,80	1.22	4 (7%)
4	PGW	D	601	-	21,21,50	0.60	0	23,23,56	1.22	3 (13%)

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	NAP	A	1001	-	-	0/27/67/67	0/5/5/5
4	PGW	B	601	-	-	0/18/18/55	0/0/0/0
4	PGW	B	602	-	-	0/2/2/55	0/0/0/0
4	PGW	B	603	-	-	0/2/2/55	0/0/0/0
4	PGW	B	604	-	-	0/2/2/55	0/0/0/0
4	PGW	B	605	-	-	0/5/5/55	0/0/0/0
4	PGW	B	606	-	-	0/4/4/55	0/0/0/0
4	PGW	B	607	-	-	0/4/4/55	0/0/0/0
4	PGW	B	608	-	-	0/21/21/55	0/0/0/0
4	PGW	B	609	-	-	0/3/3/55	0/0/0/0
4	PGW	B	610	-	-	1/31/31/55	0/0/0/0
4	PGW	B	611	-	-	0/6/6/55	0/0/0/0
4	PGW	B	612	-	-	0/3/3/55	0/0/0/0
3	NAP	C	1001	-	-	0/27/67/67	0/5/5/5
4	PGW	D	601	-	-	0/23/23/55	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	610	PGW	O01-C02	-2.16	1.43	1.46
3	A	1001	NAP	C2A-N3A	2.46	1.36	1.32
3	A	1001	NAP	C4A-N3A	2.59	1.39	1.35
3	C	1001	NAP	O4B-C1B	2.60	1.44	1.41
3	A	1001	NAP	C4N-C3N	2.89	1.44	1.39
3	C	1001	NAP	C2A-N3A	2.91	1.37	1.32
3	C	1001	NAP	C4A-N3A	2.92	1.39	1.35
3	A	1001	NAP	C6N-N1N	3.02	1.43	1.35
3	C	1001	NAP	C6N-N1N	3.22	1.44	1.35
3	C	1001	NAP	C4N-C3N	3.33	1.45	1.39
3	A	1001	NAP	O4B-C1B	3.41	1.45	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	610	PGW	O01-C1-O02	-4.31	119.78	125.50
4	B	610	PGW	C02-O01-C1	-4.17	110.25	117.29
3	C	1001	NAP	N3A-C2A-N1A	-3.89	125.92	128.89
3	A	1001	NAP	N3A-C2A-N1A	-3.77	126.00	128.89
4	B	601	PGW	C01-O03-C19	-2.68	109.52	117.02
4	D	601	PGW	C01-O03-C19	-2.46	109.97	116.85
4	B	608	PGW	C01-O03-C19	-2.18	110.75	116.85
3	A	1001	NAP	O4D-C1D-N1N	2.10	110.44	108.13
3	C	1001	NAP	C2A-N1A-C6A	2.13	122.57	118.77
3	C	1001	NAP	O4D-C1D-N1N	2.20	110.55	108.13
4	B	610	PGW	O03-C19-C20	2.22	118.66	111.90
4	B	608	PGW	O11-P-O14	2.26	112.89	107.14
3	A	1001	NAP	C2A-N1A-C6A	2.30	122.87	118.77
3	A	1001	NAP	P2B-O2B-C2B	2.30	127.08	121.56
4	B	601	PGW	O01-C1-C2	2.31	118.95	111.90
4	D	601	PGW	O03-C19-C20	2.33	118.99	111.90
4	B	601	PGW	O03-C19-C20	2.50	119.50	111.90
4	B	608	PGW	O03-C19-C20	2.89	119.46	111.21
4	B	608	PGW	O01-C1-C2	2.95	117.93	111.53
3	C	1001	NAP	PN-O3-PA	3.18	141.66	132.73
4	D	601	PGW	O01-C1-C2	3.26	118.62	111.53
3	A	1001	NAP	PN-O3-PA	3.32	142.05	132.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	610	PGW	C02-O01-C1-O02

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	NAP	2	0
4	B	601	PGW	3	0
4	B	606	PGW	1	0
4	B	608	PGW	2	0
4	B	609	PGW	1	0
4	B	610	PGW	2	0
3	C	1001	NAP	3	0
4	D	601	PGW	7	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	326/333 (97%)	-0.10	2 (0%) 90 89	22, 42, 68, 94	0
1	C	326/333 (97%)	-0.07	3 (0%) 85 84	24, 46, 77, 102	0
2	B	389/514 (75%)	0.62	49 (12%) 5 3	33, 79, 137, 146	0
2	D	318/514 (61%)	0.78	55 (17%) 2 1	39, 97, 171, 187	0
All	All	1359/1694 (80%)	0.32	109 (8%) 15 10	22, 61, 149, 187	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	269	THR	8.6
2	B	192	ASN	7.9
2	B	152	LEU	7.6
2	B	196	HIS	7.2
2	D	161	PRO	6.4
2	B	153	PHE	6.4
2	B	195	MET	6.4
2	D	168	VAL	5.4
2	D	288	VAL	5.3
2	D	205	TYR	5.3
2	B	191	GLU	5.3
1	C	360	TYR	5.2
2	D	275	SER	5.0
2	D	206	SER	4.9
2	D	237	PHE	4.8
2	D	271	PHE	4.8
2	D	235	PHE	4.7
2	D	225	VAL	4.6
1	C	36	LEU	4.6
2	D	155	TYR	4.5
2	B	193	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	158	SER	4.2
2	B	205	TYR	4.2
2	D	291	ILE	4.2
2	D	238	LEU	4.2
2	D	204	THR	4.2
2	B	204	THR	4.1
2	D	253	ASN	4.1
2	B	145	PHE	4.0
2	D	165	ILE	4.0
2	D	415	ARG	3.9
2	B	200	VAL	3.9
2	D	258	ILE	3.8
2	D	222	PHE	3.8
2	B	151	LEU	3.8
2	B	194	ASP	3.7
2	B	242	PHE	3.7
2	D	268	VAL	3.7
2	D	233	TRP	3.7
2	B	190	ASP	3.6
2	D	290	GLN	3.6
2	D	294	ILE	3.6
2	B	150	TRP	3.5
2	B	155	TYR	3.5
2	B	199	GLY	3.5
2	B	219	THR	3.5
2	D	164	ILE	3.4
2	B	215	SER	3.3
1	A	360	TYR	3.3
2	B	156	PRO	3.3
2	D	252	THR	3.2
2	B	213	GLN	3.2
2	B	214	GLN	3.2
2	D	159	SER	3.2
2	D	265	PRO	3.1
2	B	165	ILE	3.1
2	D	160	GLY	3.0
2	B	197	GLY	2.9
2	B	161	PRO	2.9
2	B	241	PHE	2.9
2	B	125	MET	2.9
2	D	189	ARG	2.8
2	D	156	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	162	ALA	2.8
2	D	267	TYR	2.7
2	D	231	ILE	2.7
2	B	154	GLU	2.7
2	B	273	THR	2.7
2	B	164	ILE	2.7
2	D	207	GLN	2.7
2	D	166	ALA	2.6
2	D	129	ASP	2.6
2	D	157	GLU	2.6
2	B	149	VAL	2.6
2	B	274	GLU	2.5
2	B	270	ILE	2.5
2	D	260	ILE	2.5
2	B	203	HIS	2.5
2	D	98	LEU	2.4
2	D	306	HIS	2.4
2	D	266	TYR	2.4
2	D	254	ILE	2.4
2	D	226	GLU	2.4
2	D	259	ASP	2.4
2	B	218	PHE	2.4
2	B	30	GLU	2.3
2	B	306	HIS	2.3
2	D	203	HIS	2.3
2	D	229	CYS	2.3
2	D	302	LYS	2.3
2	B	187	ILE	2.3
1	C	352	ASP	2.3
2	B	216	THR	2.3
2	D	221	PRO	2.3
2	B	251	PHE	2.2
2	D	344	PHE	2.2
2	B	159	SER	2.2
2	B	167	ILE	2.2
2	B	272	LEU	2.1
2	B	201	THR	2.1
2	B	120	GLU	2.1
2	B	146	GLN	2.1
2	B	285	VAL	2.1
2	D	172	VAL	2.1
2	D	239	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	228	LEU	2.0
2	D	287	ARG	2.0
1	A	349	HIS	2.0
2	D	173	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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
4	PGW	D	601	22/51	0.62	0.42	6.97	95,113,118,118	0
4	PGW	B	606	7/51	0.68	0.48	6.21	90,91,93,93	0
4	PGW	B	601	19/51	0.64	0.42	5.87	72,84,97,97	0
4	PGW	B	609	6/51	0.90	0.33	5.34	73,73,73,74	0
4	PGW	B	605	8/51	0.81	0.60	5.29	74,74,75,75	0
4	PGW	B	608	20/51	0.76	0.42	2.88	141,146,153,153	0
4	PGW	B	611	9/51	0.75	0.53	1.77	83,84,85,85	0
4	PGW	B	610	28/51	0.74	0.30	1.44	122,148,154,155	0
3	NAP	C	1001	48/48	0.98	0.18	0.19	38,45,53,54	0
3	NAP	A	1001	48/48	0.98	0.17	-0.34	35,43,47,48	0
5	K	D	503	1/1	0.98	0.34	-	41,41,41,41	1
5	K	B	501	1/1	0.98	0.39	-	32,32,32,32	1
5	K	D	501	1/1	0.76	0.41	-	37,37,37,37	1
4	PGW	B	602	5/51	0.69	0.34	-	80,81,82,82	0
5	K	D	505	1/1	0.90	0.58	-	53,53,53,53	1
4	PGW	B	604	5/51	0.80	0.30	-	87,87,88,88	0
4	PGW	B	607	7/51	0.67	0.46	-	94,96,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	K	B	503	1/1	0.94	0.31	-	28,28,28,28	1
4	PGW	B	603	5/51	0.81	0.29	-	85,87,88,88	0
4	PGW	B	612	6/51	0.60	0.55	-	94,96,96,97	0
5	K	B	505	1/1	0.86	0.41	-	64,64,64,64	1
5	K	D	502	1/1	0.87	0.32	-	34,34,34,34	1
5	K	B	504	1/1	0.96	0.34	-	26,26,26,26	1
5	K	D	504	1/1	0.98	0.39	-	26,26,26,26	1
5	K	B	502	1/1	0.89	0.34	-	21,21,21,21	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.