



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:39 AM GMT

PDB ID : 3BJQ
Title : CRYSTAL STRUCTURE OF A PHAGE-RELATED PROTEIN (BB3626)
FROM BORDETELLA BRONCHISEPTICA RB50 AT 2.05 Å RESOLU-
TION
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2007-12-04
Resolution : 2.05 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

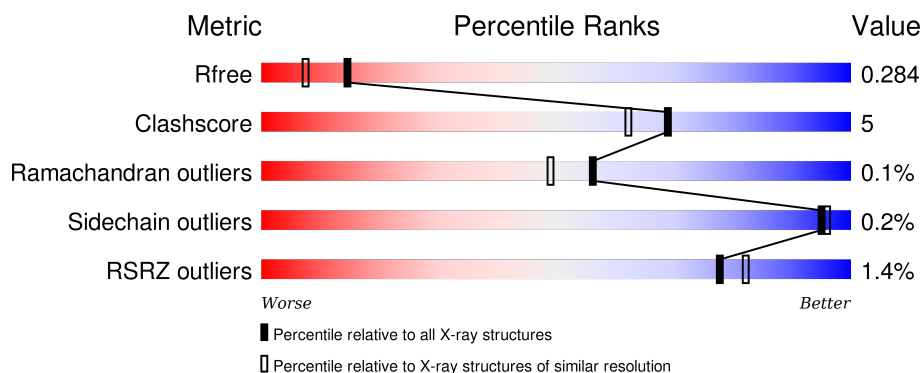
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	316	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	B	316	<div> <div></div> <div>88%</div> <div>7%</div> <div>• •</div> </div>
1	C	316	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>
1	D	316	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>• •</div> </div> </div>
1	E	316	<div> <div></div> <div>90%</div> <div>7%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	316	
1	G	316	
1	H	316	
1	I	316	
1	J	316	

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
3	PG4	B	318	-	-	-	X
3	PG4	B	319	-	-	-	X
3	PG4	E	317	-	-	-	X
3	PG4	G	318	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24467 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 Phage-related protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	Se	0	0	0
			2271	1447	385	431	2	6			
1	B	303	Total	C	N	O	S	Se	0	5	0
			2339	1491	390	449	2	7			
1	C	294	Total	C	N	O	S	Se	0	0	0
			2234	1427	375	424	2	6			
1	D	303	Total	C	N	O	S	Se	0	2	0
			2326	1483	393	442	2	6			
1	E	305	Total	C	N	O	S	Se	0	1	0
			2358	1499	403	448	2	6			
1	F	296	Total	C	N	O	S	Se	0	2	0
			2269	1446	385	430	2	6			
1	G	295	Total	C	N	O	S	Se	0	1	0
			2269	1446	386	429	2	6			
1	H	292	Total	C	N	O	S	Se	0	3	0
			2240	1434	374	424	2	6			
1	I	293	Total	C	N	O	S	Se	0	2	0
			2269	1448	387	426	2	6			
1	J	298	Total	C	N	O	S	Se	0	4	0
			2293	1463	388	434	2	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	UNP Q7WDF2
B	0	GLY	-	LEADER SEQUENCE	UNP Q7WDF2
C	0	GLY	-	LEADER SEQUENCE	UNP Q7WDF2
D	0	GLY	-	LEADER SEQUENCE	UNP Q7WDF2
E	0	GLY	-	LEADER SEQUENCE	UNP Q7WDF2
F	0	GLY	-	LEADER SEQUENCE	UNP Q7WDF2
G	0	GLY	-	LEADER SEQUENCE	UNP Q7WDF2
H	0	GLY	-	LEADER SEQUENCE	UNP Q7WDF2
I	0	GLY	-	LEADER SEQUENCE	UNP Q7WDF2

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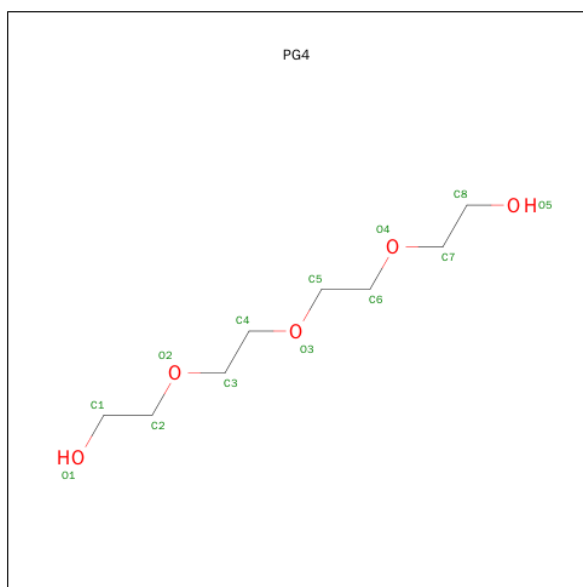
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Chain	Residue	Modelled	Actual	Comment	Reference
J	0	GLY	-	LEADER SEQUENCE	UNP Q7WDF2

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 13 8 5	0	0
3	D	1	Total C O 13 8 5	0	0
3	E	1	Total C O 13 8 5	0	0
3	F	1	Total C O 13 8 5	0	0
3	G	1	Total C O 13 8 5	0	0
3	H	1	Total C O 13 8 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total C O 13 8 5	0	0
3	J	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 10 6 4	0	0
3	D	1	Total C O 13 8 5	0	0
3	E	1	Total C O 13 8 5	0	0
3	F	1	Total C O 13 8 5	0	0
3	H	1	Total C O 7 4 3	0	0
3	I	1	Total C O 9 6 3	0	0
3	J	1	Total C O 10 6 4	0	0
3	G	1	Total C O 13 8 5	0	0
3	G	1	Total C O 10 6 4	0	0
3	B	1	Total C O 10 6 4	0	0
3	B	1	Total C O 10 6 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	143	Total O 143 143	0	0
4	B	143	Total O 143 143	0	0
4	C	84	Total O 84 84	0	0
4	D	176	Total O 176 176	0	0
4	E	172	Total O 172 172	0	0

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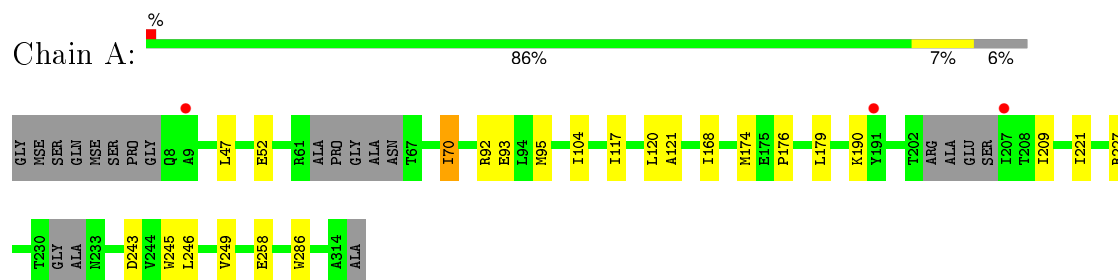
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	89	Total 89	O 89	0	0
4	G	129	Total 129	O 129	0	0
4	H	125	Total 125	O 125	0	0
4	I	122	Total 123	O 123	0	1
4	J	153	Total 153	O 153	0	0

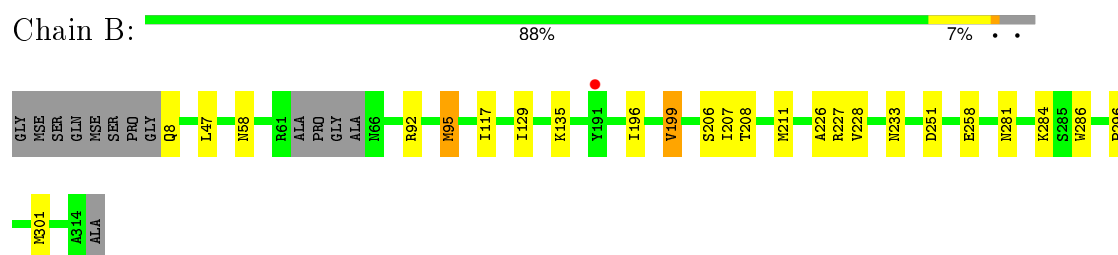
3 Residue-property plots [i](#)

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.

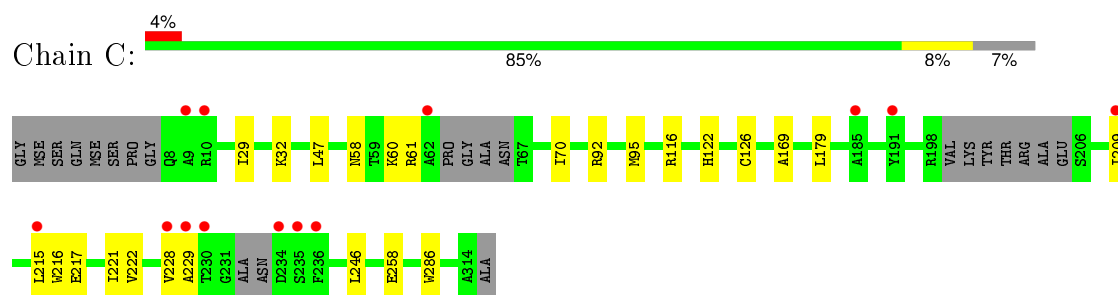
- Molecule 1: Phage-related protein



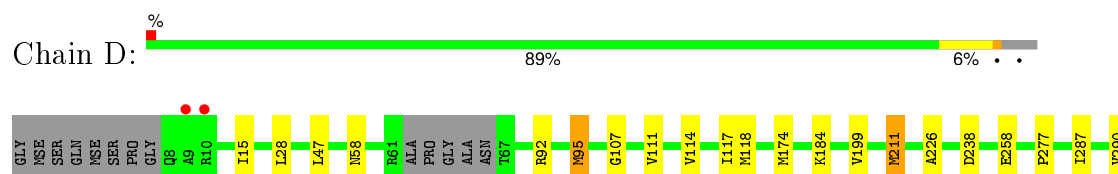
- Molecule 1: Phage-related protein



- Molecule 1: Phage-related protein



- Molecule 1: Phage-related protein





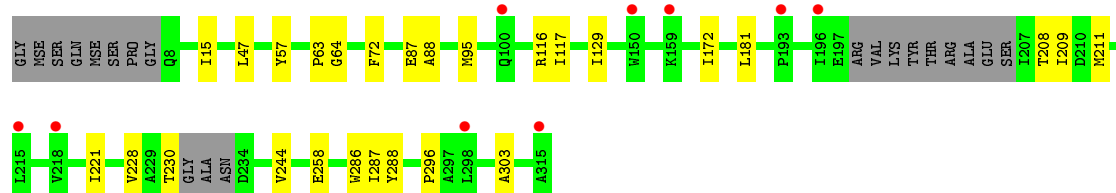
- Molecule 1: Phage-related protein

Chain E: 90% 7% 3%



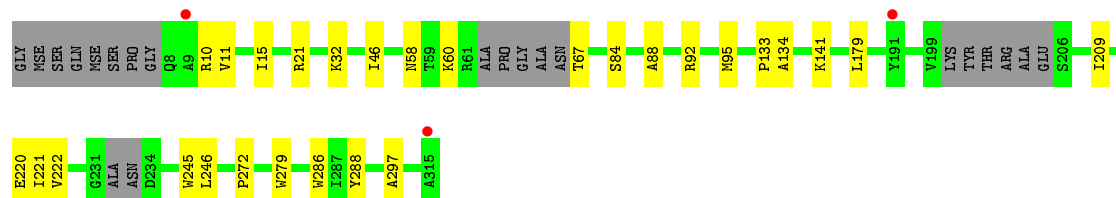
- Molecule 1: Phage-related protein

Chain F: 85% 9% 6% 3%



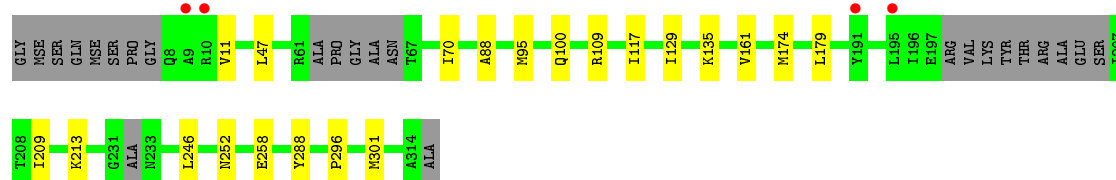
- Molecule 1: Phage-related protein

Chain G: 84% 9% 7%



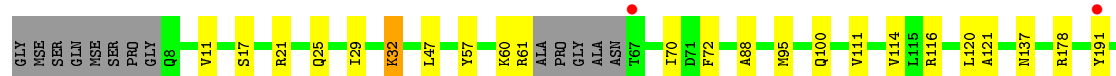
- Molecule 1: Phage-related protein

Chain H: 86% 7% 8%



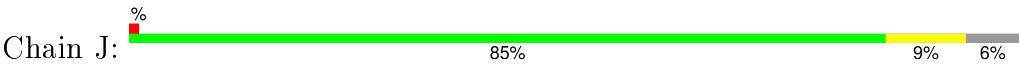
- Molecule 1: Phage-related protein

Chain I: 83% 10% 7%





● Molecule 1: Phage-related protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.39Å 188.32Å 105.15Å 90.00° 106.60° 90.00°	Depositor
Resolution (Å)	49.15 – 2.05 49.16 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.15-2.05) 99.8 (49.16-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.227 0.191 , 0.284	Depositor DCC
R_{free} test set	1728 reflections (0.80%)	DCC
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 216790 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24467	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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, 0.375 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: PG4, CL

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	0.62	0/2318	0.71	2/3145 (0.1%)
1	B	0.58	1/2404 (0.0%)	0.71	0/3267
1	C	0.51	0/2281	0.64	0/3096
1	D	0.62	1/2382 (0.0%)	0.70	1/3235 (0.0%)
1	E	0.57	0/2412	0.67	0/3273
1	F	0.51	0/2324	0.65	0/3156
1	G	0.59	0/2319	0.70	0/3143
1	H	0.58	1/2294 (0.0%)	0.68	0/3111
1	I	0.55	0/2323	0.68	0/3148
1	J	0.60	0/2353	0.71	0/3195
All	All	0.57	3/23410 (0.0%)	0.69	3/31769 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	MSE	SE-CE	-6.01	1.60	1.95
1	H	174	MSE	SE-CE	-5.88	1.60	1.95
1	D	95	MSE	SE-CE	-5.69	1.61	1.95

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	211	MSE	CG-SE-CE	-6.94	83.64	98.90
1	A	243	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	243	ASP	CB-CG-OD2	-5.25	113.57	118.30

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	2271	0	2212	25	0
1	B	2339	0	2283	22	0
1	C	2234	0	2176	28	0
1	D	2326	0	2278	19	0
1	E	2358	0	2325	15	0
1	F	2269	0	2221	25	0
1	G	2269	0	2228	27	0
1	H	2240	0	2205	23	0
1	I	2269	0	2232	25	0
1	J	2293	0	2256	36	0
2	D	1	0	0	0	0
3	A	13	0	18	0	0
3	B	46	0	62	2	0
3	C	23	0	31	2	0
3	D	26	0	36	3	0
3	E	26	0	36	4	0
3	F	26	0	36	2	0
3	G	36	0	49	4	0
3	H	20	0	27	0	0
3	I	22	0	29	2	0
3	J	23	0	31	3	0
4	A	143	0	0	2	0
4	B	143	0	0	1	0
4	C	84	0	0	2	0
4	D	176	0	0	3	0
4	E	172	0	0	4	0
4	F	89	0	0	6	0
4	G	129	0	0	1	0
4	H	125	0	0	3	0
4	I	123	0	0	2	0
4	J	153	0	0	4	0
All	All	24467	0	22771	212	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 5.

All (212) 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:117:ILE:HD11	1:C:70:ILE:HG21	1.18	1.18
1:B:207:ILE:HG23	1:B:211[B]:MSE:HE2	1.44	0.98
1:D:199:VAL:HG22	1:D:211:MSE:HE1	1.46	0.94
1:A:117:ILE:CD1	1:C:70:ILE:HG21	1.99	0.92
1:I:198[B]:ARG:HE	1:I:215:LEU:HD11	1.34	0.91
1:A:174:MSE:HG2	3:D:318:PG4:H72	1.55	0.88
1:A:117:ILE:HD11	1:C:70:ILE:CG2	2.04	0.85
1:B:207:ILE:HG23	1:B:211[B]:MSE:CE	2.08	0.83
1:D:199:VAL:HG22	1:D:211:MSE:CE	2.08	0.82
1:H:70:ILE:HG21	1:J:117:ILE:HD11	1.62	0.82
1:H:70:ILE:CG2	1:J:117:ILE:HD11	2.11	0.80
1:C:47:LEU:HD23	1:C:258:GLU:HA	1.62	0.79
1:B:117:ILE:HD11	1:E:70:ILE:HG21	1.62	0.79
1:J:137:ASN:HB3	4:J:457:HOH:O	1.83	0.78
1:F:228:VAL:CG2	4:F:399:HOH:O	2.31	0.78
1:I:47:LEU:HD23	1:I:258:GLU:HA	1.65	0.76
1:A:70:ILE:HG21	1:D:117:ILE:HD11	1.70	0.73
1:F:117:ILE:HD12	1:J:70:ILE:HG13	1.71	0.72
1:B:92:ARG:HA	1:B:95:MSE:HE3	1.72	0.71
1:J:47:LEU:HD23	1:J:258:GLU:HA	1.73	0.70
1:A:95:MSE:HE1	1:A:286:TRP:HD1	1.57	0.70
1:D:92:ARG:HA	1:D:95:MSE:HE3	1.73	0.69
1:A:179:LEU:HD13	1:A:246:LEU:HG	1.74	0.69
1:B:95:MSE:HE1	1:B:286:TRP:HD1	1.58	0.68
1:E:47:LEU:HD23	1:E:258:GLU:HA	1.75	0.68
1:J:137:ASN:HB3	4:J:417:HOH:O	1.93	0.67
1:C:95:MSE:HE1	1:C:286:TRP:CD1	2.31	0.66
1:B:208:THR:H	1:B:211[A]:MSE:HE3	1.60	0.65
1:F:228:VAL:HG21	4:F:399:HOH:O	1.94	0.65
1:B:251:ASP:OD2	4:B:403:HOH:O	2.14	0.65
1:C:95:MSE:HE1	1:C:286:TRP:HD1	1.61	0.64
1:B:206:SER:O	1:B:211[A]:MSE:HE1	1.99	0.63
1:C:92:ARG:HA	1:C:95:MSE:HE3	1.80	0.63
1:G:95:MSE:HE1	1:G:286:TRP:HD1	1.65	0.62
1:F:15:ILE:HD13	4:F:394:HOH:O	1.99	0.62
1:F:116:ARG:HH21	3:F:317:PG4:H51	1.63	0.62
1:B:228:VAL:CG1	4:E:326:HOH:O	2.47	0.61
1:J:209:ILE:HD12	1:J:221:ILE:CG2	2.29	0.61
1:A:92:ARG:HA	1:A:95:MSE:HE3	1.82	0.61
1:G:92:ARG:HA	1:G:95:MSE:HE3	1.82	0.61
1:H:179[B]:LEU:HD13	1:H:246[B]:LEU:HD13	1.83	0.61
1:F:47:LEU:HD23	1:F:258:GLU:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:MSE:HE1	1:A:286:TRP:CD1	2.37	0.60
1:A:93:GLU:OE2	4:A:435:HOH:O	2.17	0.60
1:I:198[B]:ARG:HE	1:I:215:LEU:CD1	2.12	0.59
1:J:137:ASN:CB	4:J:417:HOH:O	2.49	0.59
1:H:109:ARG:HD2	4:H:424:HOH:O	2.03	0.59
1:G:10:ARG:HG3	1:G:11:VAL:H	1.67	0.59
1:F:117:ILE:CD1	1:J:70:ILE:HG13	2.33	0.59
1:B:47:LEU:HD23	1:B:258:GLU:HA	1.83	0.59
1:B:226:ALA:HA	3:B:317:PG4:H71	1.85	0.58
1:G:209:ILE:HG23	1:G:221:ILE:HB	1.83	0.58
1:G:67:THR:N	4:G:449:HOH:O	2.36	0.58
1:F:63:PRO:HB3	1:G:84:SER:CB	2.34	0.58
1:A:209:ILE:HG23	1:A:221:ILE:HB	1.86	0.57
1:F:63:PRO:CB	1:G:84:SER:CB	2.82	0.57
1:A:179:LEU:HD13	1:A:246:LEU:CD1	2.35	0.57
1:E:105[A]:ASP:CG	4:E:400:HOH:O	2.43	0.56
1:D:47:LEU:HD23	1:D:258:GLU:HA	1.86	0.56
1:D:184:LYS:NZ	1:D:238:ASP:OD2	2.37	0.56
1:G:209:ILE:HD12	1:G:221:ILE:CG2	2.36	0.56
1:G:141:LYS:HZ2	3:G:318:PG4:H11	1.71	0.56
1:I:209:ILE:HG23	1:I:221:ILE:HB	1.88	0.55
1:G:15:ILE:H	1:G:15:ILE:HD12	1.72	0.55
1:B:135:LYS:O	1:B:301:MSE:HG3	2.06	0.55
1:H:70:ILE:HG13	1:J:117:ILE:HD12	1.89	0.55
1:C:47:LEU:CD2	1:C:258:GLU:HA	2.37	0.55
1:J:209:ILE:HD12	1:J:221:ILE:HG21	1.88	0.55
1:C:116:ARG:HH21	3:C:317:PG4:H52	1.71	0.54
1:A:227:ARG:NH2	1:C:169:ALA:HB1	2.22	0.54
1:I:116:ARG:HE	3:I:317:PG4:C6	2.20	0.54
1:H:117:ILE:HD11	1:I:70:ILE:HG21	1.90	0.54
1:B:95:MSE:HE1	1:B:286:TRP:CD1	2.40	0.53
1:J:23:TYR:HB3	3:J:316:PG4:H52	1.91	0.53
1:G:10:ARG:HG3	1:G:11:VAL:N	2.23	0.53
1:H:70:ILE:HD12	1:J:117:ILE:CD1	2.39	0.52
1:J:25:GLN:HE22	3:J:317:PG4:H61	1.74	0.52
1:J:215:LEU:HD22	1:J:216:TRP:CD1	2.45	0.52
1:F:129:ILE:HD11	4:F:391:HOH:O	2.09	0.52
1:A:179:LEU:HD13	1:A:246:LEU:CG	2.41	0.51
1:F:116:ARG:HH21	3:F:317:PG4:C5	2.21	0.51
1:H:135:LYS:O	1:H:301:MSE:HG3	2.11	0.51
1:A:117:ILE:CD1	1:C:70:ILE:HG13	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:215:LEU:O	1:J:215:LEU:HD23	2.11	0.51
1:H:70:ILE:HG23	1:J:117:ILE:HD11	1.90	0.50
1:G:209:ILE:HD12	1:G:221:ILE:HG21	1.93	0.50
1:D:107:GLY:O	1:D:111:VAL:HG23	2.11	0.50
1:D:118:MSE:HE1	4:D:326:HOH:O	2.11	0.50
1:J:227:ARG:O	3:J:317:PG4:H12	2.12	0.50
1:F:129:ILE:HD12	1:F:296:PRO:HB2	1.93	0.50
1:B:129:ILE:HD12	1:B:296:PRO:HB2	1.94	0.50
1:F:95:MSE:HE1	1:F:286:TRP:HD1	1.76	0.49
1:F:228:VAL:HG22	4:F:399:HOH:O	2.03	0.49
1:G:95:MSE:HE1	1:G:286:TRP:CD1	2.45	0.49
1:G:134:ALA:HA	3:G:318:PG4:H32	1.95	0.49
1:G:60:LYS:HG2	1:I:121:ALA:HA	1.94	0.49
1:A:179:LEU:HD12	1:A:245:TRP:O	2.13	0.49
1:I:32:LYS:NZ	1:I:220:GLU:OE2	2.45	0.49
1:F:230:THR:C	4:F:402:HOH:O	2.50	0.49
1:J:190:LYS:O	1:J:207:ILE:HD12	2.14	0.48
1:I:25:GLN:HE22	3:I:317:PG4:C6	2.26	0.48
1:G:46:ILE:HD13	1:G:297:ALA:HB1	1.95	0.48
1:B:227:ARG:HH22	1:E:169:ALA:HB1	1.79	0.48
1:J:179:LEU:HD13	1:J:246:LEU:HD13	1.96	0.48
1:E:213:LYS:HD2	4:E:412:HOH:O	2.12	0.48
1:C:179:LEU:HD13	1:C:246:LEU:CD1	2.44	0.47
1:G:58:ASN:HA	1:I:120:LEU:HD21	1.96	0.47
1:A:190:LYS:HE3	1:C:217:GLU:OE2	2.14	0.47
1:B:226:ALA:HA	3:B:317:PG4:C7	2.44	0.47
1:B:281:ASN:O	1:B:284:LYS:NZ	2.40	0.47
1:G:32:LYS:NZ	1:G:220:GLU:OE2	2.45	0.47
1:D:277:PRO:O	1:H:11:VAL:HG21	2.13	0.47
1:C:215:LEU:HD22	1:C:216:TRP:CD1	2.49	0.47
1:J:89:LYS:HD2	4:J:433:HOH:O	2.14	0.47
1:I:178:ARG:NH1	4:I:471:HOH:O	2.47	0.47
1:C:228:VAL:CG1	4:C:396:HOH:O	2.62	0.47
1:H:70:ILE:HD12	1:J:117:ILE:HD13	1.96	0.47
1:D:118:MSE:HE2	4:D:447:HOH:O	2.14	0.47
1:A:47:LEU:HD23	1:A:258:GLU:HA	1.97	0.47
1:H:129:ILE:HD12	1:H:296:PRO:HB2	1.97	0.47
1:G:179:LEU:HD13	1:G:246:LEU:HG	1.97	0.47
1:F:87:GLU:HB3	1:F:287:ILE:HG23	1.96	0.46
1:A:117:ILE:HD13	1:C:70:ILE:HG13	1.96	0.46
1:I:211:MSE:HB3	4:I:436:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:137:ASN:OD1	1:J:139:ASP:OD1	2.32	0.46
1:I:29:ILE:O	1:I:32:LYS:HB2	2.14	0.46
1:I:88:ALA:HB3	1:I:288:TYR:HB2	1.96	0.46
1:I:191[A]:TYR:HA	1:I:196:ILE:HD11	1.97	0.46
1:G:32:LYS:HG2	1:G:222:VAL:HG11	1.96	0.46
1:I:198[B]:ARG:NE	1:I:215:LEU:HD11	2.17	0.46
1:E:277:PRO:O	1:I:11:VAL:HG21	2.16	0.46
1:F:88:ALA:HB3	1:F:288:TYR:HB2	1.98	0.46
1:H:252:ASN:ND2	4:H:354:HOH:O	2.49	0.46
1:B:208:THR:HG23	1:B:211[A]:MSE:CE	2.46	0.46
1:A:120:LEU:CD2	1:C:58:ASN:HA	2.46	0.46
1:J:129:ILE:HD12	1:J:296:PRO:HB2	1.98	0.46
1:C:179:LEU:HD13	1:C:246:LEU:HD11	1.98	0.46
1:D:92:ARG:HA	1:D:95:MSE:CE	2.42	0.45
1:B:199:VAL:HG23	1:B:211[A]:MSE:SE	2.67	0.45
1:H:70:ILE:HG21	1:J:117:ILE:CD1	2.40	0.45
1:E:89:LYS:HG3	1:E:285:SER:HB3	1.99	0.45
1:C:209:ILE:HG23	1:C:221:ILE:HB	1.98	0.45
1:A:190:LYS:CE	1:C:217:GLU:OE2	2.65	0.45
1:E:226:ALA:HA	3:E:317:PG4:C7	2.47	0.45
1:H:88:ALA:HB3	1:H:288:TYR:HB2	1.98	0.45
1:D:28:LEU:HD21	3:D:318:PG4:H41	1.97	0.45
1:F:208:THR:OG1	1:F:211:MSE:HE3	2.17	0.45
1:D:174:MSE:HG2	3:E:317:PG4:H81	1.98	0.45
1:F:117:ILE:HD11	1:J:70:ILE:HG21	1.99	0.45
1:E:226:ALA:HA	3:E:317:PG4:H71	1.97	0.44
1:J:242:PRO:HG2	1:J:309:ASP:HA	1.99	0.44
1:I:17:SER:O	1:I:21:ARG:HG3	2.18	0.44
1:G:21:ARG:HG2	1:G:272:PRO:HD2	2.00	0.44
1:J:178:ARG:O	1:J:246:LEU:HD12	2.17	0.44
1:G:179:LEU:HD13	1:G:246:LEU:CD1	2.47	0.44
1:G:133:PRO:HB2	3:G:318:PG4:H11	2.00	0.44
1:A:121:ALA:HA	1:C:60:LYS:HG3	1.99	0.44
1:E:95:MSE:HE1	1:E:100:GLN:O	2.18	0.44
1:B:196:ILE:O	1:B:199:VAL:HG12	2.17	0.44
1:D:226:ALA:HA	3:D:318:PG4:H81	2.00	0.44
1:D:277:PRO:HA	1:D:287:ILE:O	2.17	0.44
1:B:58:ASN:O	1:C:228:VAL:HG13	2.17	0.44
1:C:228:VAL:HG12	1:C:229:ALA:N	2.32	0.44
1:C:29:ILE:O	1:C:32:LYS:HB2	2.18	0.44
1:J:209:ILE:HD13	1:J:209:ILE:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:183[A]:ARG:NH2	1:J:184:LYS:HZ2	2.16	0.43
1:E:178:ARG:HG3	1:E:249:VAL:CG2	2.48	0.43
1:I:137:ASN:C	1:I:137:ASN:OD1	2.57	0.43
1:F:57:TYR:HA	1:F:72:PHE:CE1	2.53	0.43
1:H:95:MSE:HE1	1:H:100:GLN:O	2.19	0.43
1:D:211:MSE:HG2	4:D:347:HOH:O	2.18	0.43
1:F:95:MSE:HE1	1:F:286:TRP:CD1	2.52	0.43
1:J:69:ARG:O	1:J:70:ILE:HD13	2.19	0.43
1:E:135:LYS:O	1:E:301:MSE:HG3	2.19	0.43
1:D:114:VAL:HG21	1:D:290:VAL:HG21	2.00	0.43
1:A:249:VAL:HG13	4:A:367:HOH:O	2.19	0.43
1:J:209:ILE:HG23	1:J:221:ILE:HB	2.00	0.42
1:C:116:ARG:HH21	3:C:317:PG4:C5	2.32	0.42
1:E:141:LYS:NZ	4:E:447:HOH:O	2.44	0.42
1:H:209:ILE:HA	1:H:209:ILE:HD13	1.86	0.42
1:F:181:LEU:HD23	1:F:244:VAL:HG22	2.01	0.42
1:H:47:LEU:HD23	1:H:258:GLU:HA	2.01	0.42
1:H:179[A]:LEU:HD12	1:H:246[A]:LEU:HD21	2.01	0.42
1:G:141:LYS:NZ	3:G:318:PG4:H31	2.35	0.42
1:E:227:ARG:O	3:E:317:PG4:H61	2.20	0.42
1:I:60:LYS:O	1:I:61:ARG:CB	2.67	0.42
1:I:95:MSE:HE1	1:I:100:GLN:O	2.19	0.42
1:F:63:PRO:HA	1:F:64:GLY:HA2	1.82	0.41
1:G:179:LEU:HD12	1:G:245:TRP:O	2.20	0.41
1:F:209:ILE:HD12	1:F:221:ILE:HG21	2.02	0.41
1:H:179[A]:LEU:HD12	1:H:246[A]:LEU:CD2	2.49	0.41
1:C:32:LYS:HG2	1:C:222:VAL:HG11	2.02	0.41
1:D:58:ASN:HD21	1:D:174:MSE:HE2	1.84	0.41
1:I:111:VAL:O	1:I:114:VAL:HG22	2.20	0.41
1:E:227:ARG:HD3	1:E:238:ASP:OD1	2.20	0.41
1:I:47:LEU:CD2	1:I:258:GLU:HA	2.43	0.41
1:J:179:LEU:HD12	1:J:245:TRP:O	2.20	0.41
1:B:8:GLN:HG3	1:G:279:TRP:CD1	2.56	0.41
1:H:161:VAL:HG13	1:H:246[A]:LEU:HD21	2.03	0.41
1:A:168:ILE:HD13	1:A:176:PRO:HB3	2.02	0.41
1:H:117:ILE:CD1	1:I:70:ILE:HG21	2.49	0.41
1:A:52:GLU:H	1:A:52:GLU:CD	2.25	0.41
1:J:135:LYS:O	1:J:301:MSE:HG3	2.21	0.40
1:F:172:ILE:HD13	1:F:303:ALA:HA	2.02	0.40
1:C:228:VAL:HG12	4:C:396:HOH:O	2.22	0.40
1:J:183[A]:ARG:NH2	1:J:184:LYS:NZ	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ILE:H	1:D:15:ILE:HD12	1.87	0.40
1:C:122:HIS:CE1	1:C:126:CYS:SG	3.14	0.40
1:I:57:TYR:HA	1:I:72:PHE:CE1	2.56	0.40
1:J:25:GLN:HG2	1:J:28:LEU:HD12	2.04	0.40
1:G:88:ALA:HB3	1:G:288:TYR:HB2	2.04	0.40
1:H:213:LYS:HD2	4:H:383:HOH:O	2.21	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	288/316 (91%)	282 (98%)	6 (2%)	0	100	100
1	B	304/316 (96%)	298 (98%)	5 (2%)	1 (0%)	46	36
1	C	286/316 (90%)	281 (98%)	4 (1%)	1 (0%)	46	36
1	D	301/316 (95%)	294 (98%)	7 (2%)	0	100	100
1	E	302/316 (96%)	296 (98%)	5 (2%)	1 (0%)	46	36
1	F	292/316 (92%)	288 (99%)	4 (1%)	0	100	100
1	G	288/316 (91%)	281 (98%)	7 (2%)	0	100	100
1	H	287/316 (91%)	283 (99%)	4 (1%)	0	100	100
1	I	287/316 (91%)	283 (99%)	4 (1%)	0	100	100
1	J	296/316 (94%)	292 (99%)	4 (1%)	0	100	100
All	All	2931/3160 (93%)	2878 (98%)	50 (2%)	3 (0%)	56	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	ASN

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Mol	Chain	Res	Type
1	C	61	ARG
1	E	203	ARG

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	236/249 (95%)	234 (99%)	2 (1%)	86	86
1	B	246/249 (99%)	245 (100%)	1 (0%)	93	94
1	C	231/249 (93%)	231 (100%)	0	100	100
1	D	242/249 (97%)	242 (100%)	0	100	100
1	E	248/249 (100%)	247 (100%)	1 (0%)	93	94
1	F	236/249 (95%)	236 (100%)	0	100	100
1	G	237/249 (95%)	237 (100%)	0	100	100
1	H	235/249 (94%)	235 (100%)	0	100	100
1	I	237/249 (95%)	236 (100%)	1 (0%)	93	94
1	J	240/249 (96%)	240 (100%)	0	100	100
All	All	2388/2490 (96%)	2383 (100%)	5 (0%)	95	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ILE
1	A	104	ILE
1	B	199	VAL
1	E	117	ILE
1	I	32	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	PG4	A	316	-	12,12,12	0.44	0	11,11,11	0.44	0
3	PG4	B	316	-	12,12,12	0.46	0	11,11,11	0.53	0
3	PG4	B	317	-	12,12,12	0.44	0	11,11,11	0.82	0
3	PG4	B	318	-	9,9,12	0.52	0	8,8,11	0.36	0
3	PG4	B	319	-	9,9,12	0.52	0	8,8,11	0.33	0
3	PG4	C	316	-	12,12,12	0.38	0	11,11,11	0.33	0
3	PG4	C	317	-	9,9,12	0.43	0	8,8,11	0.52	0
3	PG4	D	317	-	12,12,12	0.35	0	11,11,11	0.53	0
3	PG4	D	318	-	12,12,12	0.44	0	11,11,11	0.37	0
3	PG4	E	316	-	12,12,12	0.37	0	11,11,11	0.47	0
3	PG4	E	317	-	12,12,12	0.57	0	11,11,11	0.95	0
3	PG4	F	316	-	12,12,12	0.41	0	11,11,11	0.49	0
3	PG4	F	317	-	12,12,12	0.55	0	11,11,11	0.52	0
3	PG4	G	316	-	12,12,12	0.36	0	11,11,11	0.54	0
3	PG4	G	317	-	12,12,12	0.52	0	11,11,11	0.25	0
3	PG4	G	318	-	9,9,12	0.51	0	8,8,11	0.49	0
3	PG4	H	316	-	12,12,12	0.43	0	11,11,11	0.41	0
3	PG4	H	317	-	6,6,12	0.52	0	5,5,11	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PG4	I	316	-	12,12,12	0.49	0	11,11,11	0.22	0
3	PG4	I	317	-	8,8,12	0.65	0	7,7,11	0.46	0
3	PG4	J	316	-	12,12,12	0.39	0	11,11,11	0.37	0
3	PG4	J	317	-	9,9,12	0.47	0	8,8,11	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG4	A	316	-	-	0/10/10/10	0/0/0/0
3	PG4	B	316	-	-	0/10/10/10	0/0/0/0
3	PG4	B	317	-	-	0/10/10/10	0/0/0/0
3	PG4	B	318	-	-	0/7/7/10	0/0/0/0
3	PG4	B	319	-	-	0/7/7/10	0/0/0/0
3	PG4	C	316	-	-	0/10/10/10	0/0/0/0
3	PG4	C	317	-	-	0/7/7/10	0/0/0/0
3	PG4	D	317	-	-	0/10/10/10	0/0/0/0
3	PG4	D	318	-	-	0/10/10/10	0/0/0/0
3	PG4	E	316	-	-	0/10/10/10	0/0/0/0
3	PG4	E	317	-	-	0/10/10/10	0/0/0/0
3	PG4	F	316	-	-	0/10/10/10	0/0/0/0
3	PG4	F	317	-	-	0/10/10/10	0/0/0/0
3	PG4	G	316	-	-	0/10/10/10	0/0/0/0
3	PG4	G	317	-	-	0/10/10/10	0/0/0/0
3	PG4	G	318	-	-	0/7/7/10	0/0/0/0
3	PG4	H	316	-	-	0/10/10/10	0/0/0/0
3	PG4	H	317	-	-	0/4/4/10	0/0/0/0
3	PG4	I	316	-	-	0/10/10/10	0/0/0/0
3	PG4	I	317	-	-	0/6/6/10	0/0/0/0
3	PG4	J	316	-	-	0/10/10/10	0/0/0/0
3	PG4	J	317	-	-	0/7/7/10	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	317	PG4	2	0
3	C	317	PG4	2	0
3	D	318	PG4	3	0
3	E	317	PG4	4	0
3	F	317	PG4	2	0
3	G	318	PG4	4	0
3	I	317	PG4	2	0
3	J	316	PG4	1	0
3	J	317	PG4	2	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	290/316 (91%)	-0.20	3 (1%) 84 87	24, 39, 62, 85	0
1	B	297/316 (93%)	-0.16	1 (0%) 94 95	26, 39, 58, 75	0
1	C	288/316 (91%)	0.20	13 (4%) 37 42	33, 49, 82, 97	0
1	D	297/316 (93%)	-0.31	2 (0%) 89 91	24, 37, 52, 74	0
1	E	299/316 (94%)	-0.23	1 (0%) 94 95	27, 38, 50, 73	0
1	F	290/316 (91%)	0.38	9 (3%) 52 60	31, 48, 79, 95	0
1	G	289/316 (91%)	-0.13	3 (1%) 84 87	26, 41, 63, 82	0
1	H	286/316 (90%)	-0.10	4 (1%) 78 82	27, 41, 63, 82	0
1	I	287/316 (90%)	-0.12	3 (1%) 84 87	28, 41, 58, 76	0
1	J	292/316 (92%)	-0.25	2 (0%) 89 91	23, 38, 59, 80	0
All	All	2915/3160 (92%)	-0.09	41 (1%) 78 82	23, 41, 67, 97	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	ALA	10.4
1	F	315	ALA	5.1
1	G	191	TYR	4.7
1	C	191	TYR	4.4
1	C	236	PHE	4.1
1	G	315	ALA	3.8
1	C	235	SER	3.5
1	H	195	LEU	3.4
1	H	191	TYR	3.3
1	C	230	THR	3.3
1	I	67	THR	3.2
1	F	159	LYS	3.1
1	C	209	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	191[A]	TYR	3.0
1	C	10	ARG	2.9
1	G	9	ALA	2.9
1	C	62	ALA	2.8
1	F	150	TRP	2.7
1	D	10	ARG	2.6
1	F	193	PRO	2.6
1	C	229	ALA	2.4
1	A	207	ILE	2.4
1	C	234	ASP	2.4
1	J	191	TYR	2.4
1	C	228	VAL	2.3
1	C	185	ALA	2.3
1	J	195	LEU	2.3
1	D	9	ALA	2.3
1	E	315	ALA	2.2
1	H	9	ALA	2.2
1	I	198[A]	ARG	2.2
1	H	10	ARG	2.2
1	F	196	ILE	2.2
1	F	298	LEU	2.1
1	A	9	ALA	2.1
1	F	100	GLN	2.1
1	C	215	LEU	2.1
1	A	191	TYR	2.0
1	F	215	LEU	2.0
1	B	191	TYR	2.0
1	F	218	VAL	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(Å ²)	Q<0.9
3	PG4	B	318	10/13	0.69	0.25	5.44	65,72,78,80	0
3	PG4	G	318	10/13	0.92	0.18	4.66	49,56,69,74	0
3	PG4	E	317	13/13	0.93	0.15	2.40	31,37,51,53	0
3	PG4	B	319	10/13	0.87	0.20	2.32	57,64,68,68	0
3	PG4	D	318	13/13	0.94	0.15	1.91	36,44,52,55	0
3	PG4	F	317	13/13	0.87	0.14	1.28	45,51,58,61	0
3	PG4	J	316	13/13	0.95	0.11	0.75	24,33,51,51	0
3	PG4	C	316	13/13	0.91	0.13	0.71	38,46,60,68	0
3	PG4	E	316	13/13	0.96	0.12	0.61	32,38,50,53	0
3	PG4	H	317	7/13	0.91	0.13	0.56	42,50,57,59	0
3	PG4	D	317	13/13	0.95	0.10	0.14	29,35,42,42	0
3	PG4	C	317	10/13	0.88	0.12	-0.24	56,60,66,66	0
3	PG4	G	316	13/13	0.97	0.09	-0.26	30,39,43,44	0
3	PG4	A	316	13/13	0.95	0.09	-0.34	27,37,47,53	0
3	PG4	J	317	10/13	0.94	0.10	-0.42	38,44,51,52	0
3	PG4	I	316	13/13	0.95	0.10	-0.45	33,39,52,55	0
3	PG4	F	316	13/13	0.95	0.10	-0.49	30,42,50,53	0
3	PG4	I	317	9/13	0.91	0.10	-0.69	38,42,49,51	0
3	PG4	H	316	13/13	0.97	0.09	-0.85	31,37,48,50	0
3	PG4	B	316	13/13	0.97	0.08	-1.64	19,31,48,48	0
3	PG4	B	317	13/13	0.96	0.09	-1.65	36,41,50,50	0
2	CL	D	316	1/1	0.91	0.08	-	59,59,59,59	0
3	PG4	G	317	13/13	0.83	0.17	-	60,67,80,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.