



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:29 PM GMT

PDB ID : 3RBQ
Title : Co-crystal structure of human UNC119 (retina gene 4) and an N-terminal Transducin-alpha mimicking peptide
Authors : Constantine, R.; Whitby, F.G.; Hill, C.P.; Baehr, W.
Deposited on : 2011-03-29
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

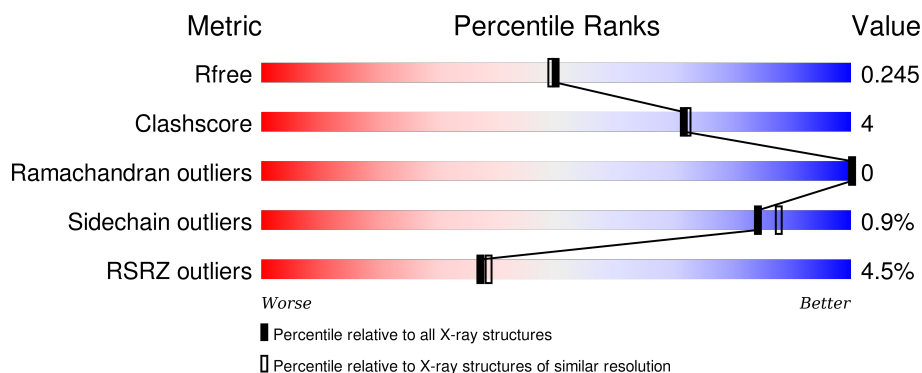
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	195	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>14%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	195	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>8%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	195	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>6%</div> <div>•</div> <div>15%</div> </div> </div>
1	D	195	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>9%</div> <div>•</div> <div>15%</div> </div> </div>
1	E	195	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>7%</div> <div>•</div> <div>15%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	195	
2	G	11	
2	H	11	
2	I	11	
2	J	11	
2	K	11	
2	L	11	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9360 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 Protein unc-119 homolog A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	3	0
			1397	898	238	254	7			
1	B	165	Total	C	N	O	S	0	1	0
			1382	889	235	251	7			
1	C	165	Total	C	N	O	S	0	2	0
			1389	894	236	252	7			
1	D	165	Total	C	N	O	S	0	2	0
			1389	894	236	252	7			
1	E	165	Total	C	N	O	S	0	0	0
			1371	883	231	250	7			
1	F	165	Total	C	N	O	S	0	0	0
			1371	883	231	250	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	MET	-	EXPRESSION TAG	UNP Q13432
A	47	GLY	-	EXPRESSION TAG	UNP Q13432
A	48	HIS	-	EXPRESSION TAG	UNP Q13432
A	49	HIS	-	EXPRESSION TAG	UNP Q13432
A	50	HIS	-	EXPRESSION TAG	UNP Q13432
A	51	HIS	-	EXPRESSION TAG	UNP Q13432
A	52	HIS	-	EXPRESSION TAG	UNP Q13432
A	53	HIS	-	EXPRESSION TAG	UNP Q13432
A	54	SER	-	EXPRESSION TAG	UNP Q13432
A	55	HIS	-	EXPRESSION TAG	UNP Q13432
B	46	MET	-	EXPRESSION TAG	UNP Q13432
B	47	GLY	-	EXPRESSION TAG	UNP Q13432
B	48	HIS	-	EXPRESSION TAG	UNP Q13432
B	49	HIS	-	EXPRESSION TAG	UNP Q13432
B	50	HIS	-	EXPRESSION TAG	UNP Q13432
B	51	HIS	-	EXPRESSION TAG	UNP Q13432
B	52	HIS	-	EXPRESSION TAG	UNP Q13432

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Chain	Residue	Modelled	Actual	Comment	Reference
B	53	HIS	-	EXPRESSION TAG	UNP Q13432
B	54	SER	-	EXPRESSION TAG	UNP Q13432
B	55	HIS	-	EXPRESSION TAG	UNP Q13432
C	46	MET	-	EXPRESSION TAG	UNP Q13432
C	47	GLY	-	EXPRESSION TAG	UNP Q13432
C	48	HIS	-	EXPRESSION TAG	UNP Q13432
C	49	HIS	-	EXPRESSION TAG	UNP Q13432
C	50	HIS	-	EXPRESSION TAG	UNP Q13432
C	51	HIS	-	EXPRESSION TAG	UNP Q13432
C	52	HIS	-	EXPRESSION TAG	UNP Q13432
C	53	HIS	-	EXPRESSION TAG	UNP Q13432
C	54	SER	-	EXPRESSION TAG	UNP Q13432
C	55	HIS	-	EXPRESSION TAG	UNP Q13432
D	46	MET	-	EXPRESSION TAG	UNP Q13432
D	47	GLY	-	EXPRESSION TAG	UNP Q13432
D	48	HIS	-	EXPRESSION TAG	UNP Q13432
D	49	HIS	-	EXPRESSION TAG	UNP Q13432
D	50	HIS	-	EXPRESSION TAG	UNP Q13432
D	51	HIS	-	EXPRESSION TAG	UNP Q13432
D	52	HIS	-	EXPRESSION TAG	UNP Q13432
D	53	HIS	-	EXPRESSION TAG	UNP Q13432
D	54	SER	-	EXPRESSION TAG	UNP Q13432
D	55	HIS	-	EXPRESSION TAG	UNP Q13432
E	46	MET	-	EXPRESSION TAG	UNP Q13432
E	47	GLY	-	EXPRESSION TAG	UNP Q13432
E	48	HIS	-	EXPRESSION TAG	UNP Q13432
E	49	HIS	-	EXPRESSION TAG	UNP Q13432
E	50	HIS	-	EXPRESSION TAG	UNP Q13432
E	51	HIS	-	EXPRESSION TAG	UNP Q13432
E	52	HIS	-	EXPRESSION TAG	UNP Q13432
E	53	HIS	-	EXPRESSION TAG	UNP Q13432
E	54	SER	-	EXPRESSION TAG	UNP Q13432
E	55	HIS	-	EXPRESSION TAG	UNP Q13432
F	46	MET	-	EXPRESSION TAG	UNP Q13432
F	47	GLY	-	EXPRESSION TAG	UNP Q13432
F	48	HIS	-	EXPRESSION TAG	UNP Q13432
F	49	HIS	-	EXPRESSION TAG	UNP Q13432
F	50	HIS	-	EXPRESSION TAG	UNP Q13432
F	51	HIS	-	EXPRESSION TAG	UNP Q13432
F	52	HIS	-	EXPRESSION TAG	UNP Q13432
F	53	HIS	-	EXPRESSION TAG	UNP Q13432
F	54	SER	-	EXPRESSION TAG	UNP Q13432

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Chain	Residue	Modelled	Actual	Comment	Reference
F	55	HIS	-	EXPRESSION TAG	UNP Q13432

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(t) subunit alpha-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	8	Total	C	N	O	0	0	0
			51	33	7	11			
2	H	9	Total	C	N	O	0	0	0
			60	38	8	14			
2	I	5	Total	C	N	O	0	0	0
			31	22	4	5			
2	J	5	Total	C	N	O	0	0	0
			31	22	4	5			
2	K	4	Total	C	N	O	0	0	0
			26	19	3	4			
2	L	10	Total	C	N	O	0	0	0
			69	44	10	15			

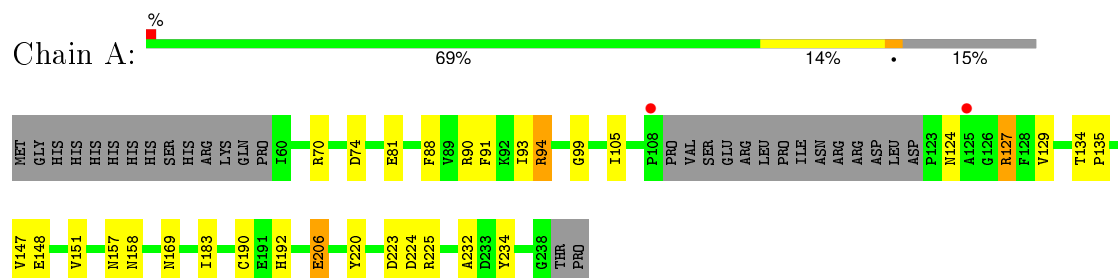
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	171	Total	O	0	0
			171	171		
3	B	132	Total	O	0	0
			132	132		
3	C	137	Total	O	0	0
			137	137		
3	D	149	Total	O	0	0
			149	149		
3	E	104	Total	O	0	0
			104	104		
3	F	93	Total	O	0	0
			93	93		
3	G	1	Total	O	0	0
			1	1		
3	H	3	Total	O	0	0
			3	3		
3	L	3	Total	O	0	0
			3	3		

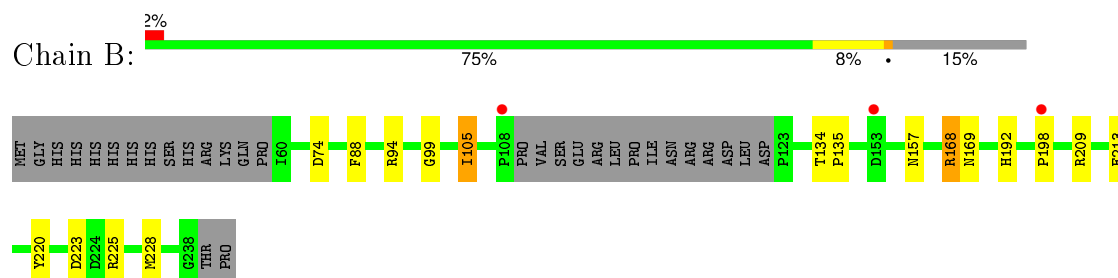
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

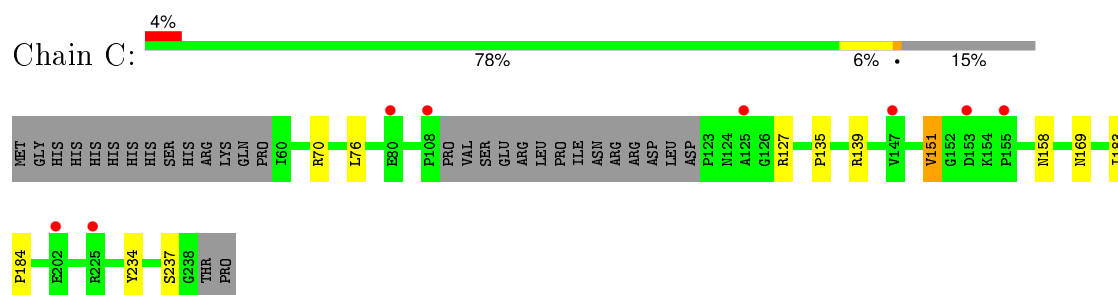
- Molecule 1: Protein unc-119 homolog A



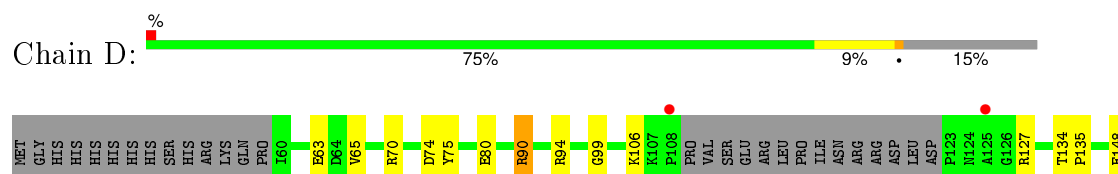
- Molecule 1: Protein unc-119 homolog A

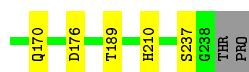


- Molecule 1: Protein unc-119 homolog A

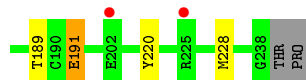
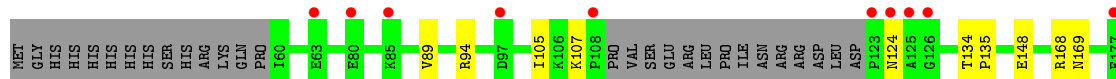
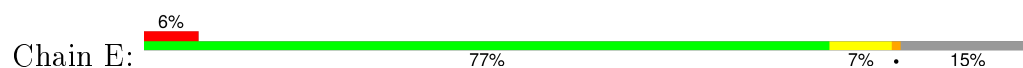


- Molecule 1: Protein unc-119 homolog A

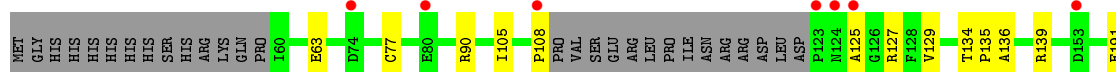
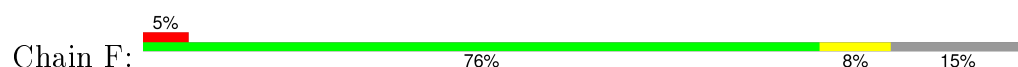




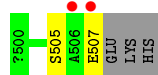
- Molecule 1: Protein unc-119 homolog A



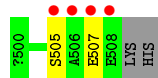
- Molecule 1: Protein unc-119 homolog A



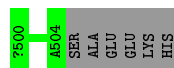
- Molecule 2: Guanine nucleotide-binding protein G(t) subunit alpha-1



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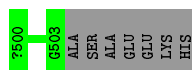


- Molecule 2: Guanine nucleotide-binding protein G(t) subunit alpha-1

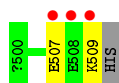




- Molecule 2: Guanine nucleotide-binding protein G(t) subunit alpha-1



- Molecule 2: Guanine nucleotide-binding protein G(t) subunit alpha-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.55Å 79.71Å 189.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.37 – 2.00 29.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.37-2.00) 100.0 (29.37-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.188 , 0.246 0.189 , 0.245	Depositor DCC
R_{free} test set	4087 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 81117 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9360	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.52% 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: DAO

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	1.27	8/1435 (0.6%)	1.04	2/1935 (0.1%)
1	B	1.10	0/1420	0.95	4/1914 (0.2%)
1	C	1.14	1/1427 (0.1%)	0.94	2/1924 (0.1%)
1	D	1.20	2/1427 (0.1%)	1.00	4/1924 (0.2%)
1	E	1.03	0/1409	0.89	0/1900
1	F	1.01	0/1409	0.85	0/1900
2	G	1.23	0/37	1.05	0/48
2	H	1.02	0/46	0.81	0/60
2	I	1.43	0/17	0.91	0/21
2	J	1.53	0/17	0.70	0/21
2	K	0.97	0/12	0.85	0/14
2	L	0.92	0/55	0.67	0/71
All	All	1.13	11/8711 (0.1%)	0.94	12/11732 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	TYR	CD1-CE1	7.88	1.51	1.39
1	A	206	GLU	CG-CD	6.37	1.61	1.51
1	A	81	GLU	CB-CG	6.31	1.64	1.52
1	A	190	CYS	CB-SG	6.13	1.92	1.82
1	A	94[A]	ARG	CG-CD	6.01	1.67	1.51
1	A	94[B]	ARG	CG-CD	6.01	1.67	1.51
1	A	234	TYR	CE1-CZ	5.96	1.46	1.38
1	D	65	VAL	CB-CG2	5.60	1.64	1.52
1	D	63	GLU	CG-CD	5.54	1.60	1.51
1	A	151	VAL	CB-CG2	5.27	1.64	1.52
1	C	234	TYR	CD2-CE2	5.01	1.46	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	ARG	C-N-CA	-7.30	103.45	121.70
1	C	127	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	B	74	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	127	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	D	74	ASP	CB-CG-OD1	6.53	124.17	118.30
1	A	74	ASP	CB-CG-OD1	6.34	124.00	118.30
1	D	127	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	169	ASN	CB-CA-C	5.75	121.90	110.40
1	C	139	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	D	176	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	90	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	209	ARG	NE-CZ-NH2	-5.15	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1397	0	1344	24	0
1	B	1382	0	1331	10	0
1	C	1389	0	1339	5	0
1	D	1389	0	1339	13	0
1	E	1371	0	1319	9	0
1	F	1371	0	1319	12	1
2	G	51	0	54	4	0
2	H	60	0	60	2	0
2	I	31	0	38	0	0
2	J	31	0	38	0	0
2	K	26	0	33	0	0
2	L	69	0	73	4	0
3	A	171	0	0	6	1
3	B	132	0	0	3	0
3	C	137	0	0	2	0
3	D	149	0	0	5	1
3	E	104	0	0	3	0
3	F	93	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	1	0
3	H	3	0	0	0	0
3	L	3	0	0	0	0
All	All	9360	0	8287	72	2

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 (72) 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)
3:A:784:HOH:O	2:G:505:SER:HB2	1.62	0.99
1:B:198:PRO:HB2	1:F:108:PRO:HB3	1.58	0.85
2:G:505:SER:OG	3:G:776:HOH:O	2.00	0.79
1:D:70:ARG:NH1	3:D:543:HOH:O	2.07	0.78
1:A:192:HIS:HD2	3:A:771:HOH:O	1.66	0.77
1:F:134:THR:HG22	1:F:136:ALA:H	1.52	0.74
1:A:206:GLU:HG2	3:A:786:HOH:O	1.91	0.69
1:B:94[A]:ARG:HE	1:B:99:GLY:HA2	1.59	0.68
1:B:225:ARG:NE	3:B:694:HOH:O	2.27	0.67
1:A:91:PHE:HD1	1:A:147[B]:VAL:HG12	1.60	0.66
1:A:88:PHE:HB2	2:G:505:SER:HB3	1.79	0.65
1:A:105:ILE:HD11	2:G:507:GLU:OE1	1.98	0.64
1:D:134:THR:HB	1:D:135:PRO:HD2	1.83	0.61
1:A:91:PHE:CD1	1:A:147[B]:VAL:HG12	2.35	0.60
1:A:124:ASN:O	1:A:127:ARG:HD3	2.02	0.59
1:F:135:PRO:HD3	1:F:236:TYR:O	2.03	0.59
1:B:157:ASN:HB2	3:B:773:HOH:O	2.05	0.57
1:A:94[A]:ARG:HH21	1:A:99:GLY:HA2	1.69	0.56
1:A:147[B]:VAL:O	1:A:147[B]:VAL:HG23	2.05	0.56
1:E:168:ARG:HD3	3:E:264:HOH:O	2.06	0.55
1:D:210:HIS:HE1	3:D:770:HOH:O	1.89	0.55
1:A:70:ARG:HG2	1:A:169:ASN:HB3	1.88	0.54
1:B:192:HIS:ND1	3:B:250:HOH:O	2.33	0.54
1:D:210:HIS:CE1	3:D:770:HOH:O	2.62	0.53
1:A:134:THR:HB	1:A:135:PRO:HD2	1.90	0.53
1:B:134:THR:HB	1:B:135:PRO:HD2	1.90	0.52
1:E:169:ASN:HA	3:E:242:HOH:O	2.10	0.52
1:A:183:ILE:HD11	1:D:75:TYR:HE2	1.75	0.51
1:E:124:ASN:ND2	3:E:656:HOH:O	2.41	0.51
1:A:94[A]:ARG:O	1:A:94[A]:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:VAL:HG13	1:E:107:LYS:HB2	1.94	0.50
1:F:77:CYS:O	1:F:127:ARG:NH1	2.30	0.49
1:C:135:PRO:HG3	1:D:135:PRO:HG3	1.94	0.49
1:A:147[B]:VAL:O	1:A:147[B]:VAL:CG2	2.61	0.49
1:E:89:VAL:O	1:E:89:VAL:HG12	2.13	0.48
1:B:88:PHE:HB2	2:H:505:SER:HB2	1.95	0.48
1:F:105:ILE:HG12	2:L:507:GLU:CG	2.43	0.48
1:F:90:ARG:HD2	3:F:664:HOH:O	2.13	0.48
1:C:70:ARG:HB2	1:C:169:ASN:CG	2.34	0.47
1:E:94:ARG:NH1	1:E:191:GLU:OE2	2.47	0.47
1:B:168:ARG:CZ	1:B:213:GLU:OE1	2.63	0.47
1:F:125:ALA:HA	2:L:509:LYS:HE3	1.97	0.47
1:A:90:ARG:HB3	1:A:148:GLU:HB2	1.97	0.47
1:A:157:ASN:ND2	1:A:158[B]:ASN:OD1	2.48	0.47
1:F:139:ARG:HD3	3:F:251:HOH:O	2.14	0.46
1:A:94[B]:ARG:HD3	3:A:286:HOH:O	2.14	0.46
1:D:170:GLN:HG3	3:D:262:HOH:O	2.16	0.46
1:D:80:GLU:N	1:D:80:GLU:CD	2.69	0.46
1:A:225:ARG:HD2	3:A:291:HOH:O	2.16	0.46
1:B:105:ILE:HD13	2:H:507:GLU:HG2	1.98	0.45
3:C:768:HOH:O	1:D:237:SER:HB3	2.16	0.45
1:D:148:GLU:HG2	1:D:189:THR:HG22	1.99	0.45
1:D:90:ARG:HD2	1:D:106:LYS:HE2	1.97	0.45
1:A:94[A]:ARG:HH21	1:A:99:GLY:CA	2.30	0.45
1:C:183:ILE:HD12	3:C:761:HOH:O	2.17	0.44
1:E:220:TYR:HB2	1:E:228:MET:HB2	1.99	0.44
1:F:63:GLU:H	1:F:63:GLU:HG2	1.56	0.44
1:D:80:GLU:H	1:D:80:GLU:CD	2.21	0.44
1:D:94[B]:ARG:NH1	1:D:99:GLY:HA2	2.33	0.43
1:B:220:TYR:HB2	1:B:228:MET:HB2	2.01	0.43
1:C:151:VAL:HG12	1:C:184:PRO:HA	2.01	0.42
1:A:124:ASN:O	1:A:127:ARG:CD	2.67	0.42
1:C:237:SER:HB3	3:D:782:HOH:O	2.18	0.42
1:F:129:VAL:O	1:F:232:ALA:HA	2.19	0.42
1:A:93:ILE:HD13	1:A:93:ILE:HG21	1.76	0.42
1:A:129:VAL:O	1:A:232:ALA:HA	2.20	0.42
1:F:125:ALA:HA	2:L:509:LYS:CE	2.50	0.41
1:F:105:ILE:HG12	2:L:507:GLU:HG3	2.01	0.41
1:A:223:ASP:O	1:A:224:ASP:HB2	2.20	0.41
1:E:134:THR:HB	1:E:135:PRO:HD2	2.02	0.41
1:A:94[A]:ARG:NH2	3:A:247:HOH:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:GLU:HG2	1:E:189:THR:HG23	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:ARG:NH1	3:F:751:HOH:O[3_654]	1.97	0.23
3:A:697:HOH:O	3:D:520:HOH:O[4_445]	2.00	0.20

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	164/195 (84%)	160 (98%)	4 (2%)	0	100	100
1	B	162/195 (83%)	160 (99%)	2 (1%)	0	100	100
1	C	163/195 (84%)	159 (98%)	4 (2%)	0	100	100
1	D	163/195 (84%)	161 (99%)	2 (1%)	0	100	100
1	E	161/195 (83%)	156 (97%)	5 (3%)	0	100	100
1	F	161/195 (83%)	157 (98%)	4 (2%)	0	100	100
2	G	5/11 (46%)	5 (100%)	0	0	100	100
2	H	6/11 (54%)	6 (100%)	0	0	100	100
2	I	2/11 (18%)	2 (100%)	0	0	100	100
2	J	2/11 (18%)	2 (100%)	0	0	100	100
2	K	1/11 (9%)	1 (100%)	0	0	100	100
2	L	7/11 (64%)	7 (100%)	0	0	100	100
All	All	997/1236 (81%)	976 (98%)	21 (2%)	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	155/181 (86%)	155 (100%)	0	100	100
1	B	153/181 (84%)	151 (99%)	2 (1%)	76	79
1	C	154/181 (85%)	151 (98%)	3 (2%)	65	67
1	D	154/181 (85%)	154 (100%)	0	100	100
1	E	152/181 (84%)	150 (99%)	2 (1%)	76	79
1	F	152/181 (84%)	151 (99%)	1 (1%)	88	91
2	G	2/5 (40%)	2 (100%)	0	100	100
2	H	3/5 (60%)	3 (100%)	0	100	100
2	L	4/5 (80%)	4 (100%)	0	100	100
All	All	929/1101 (84%)	921 (99%)	8 (1%)	84	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	105	ILE
1	B	223	ASP
1	C	76	LEU
1	C	151	VAL
1	C	158	ASN
1	E	105	ILE
1	E	191	GLU
1	F	191	GLU

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 [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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	165/195 (84%)	-0.06	2 (1%) 81 81	15, 23, 37, 56	0
1	B	165/195 (84%)	0.06	3 (1%) 71 72	18, 28, 43, 52	0
1	C	165/195 (84%)	0.21	8 (4%) 34 36	16, 28, 47, 57	0
1	D	165/195 (84%)	-0.05	2 (1%) 81 81	14, 24, 36, 55	0
1	E	165/195 (84%)	0.37	12 (7%) 18 19	19, 35, 47, 74	0
1	F	165/195 (84%)	0.43	10 (6%) 25 26	18, 35, 50, 71	0
2	G	7/11 (63%)	1.12	2 (28%) 1 1	22, 29, 55, 65	0
2	H	8/11 (72%)	2.32	4 (50%) 0 1	25, 35, 66, 70	0
2	I	4/11 (36%)	0.15	0 100 100	22, 23, 25, 28	0
2	J	4/11 (36%)	-0.02	0 100 100	27, 28, 28, 32	0
2	K	3/11 (27%)	0.60	0 100 100	46, 46, 50, 51	0
2	L	9/11 (81%)	1.63	3 (33%) 0 1	34, 45, 72, 73	0
All	All	1025/1236 (82%)	0.20	46 (4%) 37 38	14, 28, 48, 74	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	125	ALA	7.8
1	F	124	ASN	6.4
1	E	123	PRO	6.4
1	F	123	PRO	6.3
2	H	506	ALA	6.2
2	H	508	GLU	6.0
1	A	108	PRO	5.4
1	F	125	ALA	5.4
1	E	108	PRO	4.9
2	L	509	LYS	4.8
1	E	124	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
2	G	507	GLU	4.3
1	C	108	PRO	4.2
1	C	125	ALA	4.1
1	C	153	ASP	3.9
1	A	125	ALA	3.9
1	B	108	PRO	3.7
2	H	505	SER	3.7
2	L	507	GLU	3.5
1	D	108	PRO	3.4
1	E	202	GLU	3.4
2	H	507	GLU	3.3
1	E	80	GLU	3.1
1	F	80	GLU	3.0
1	C	155	PRO	3.0
1	F	153	ASP	2.9
2	L	508	GLU	2.9
2	G	506	ALA	2.8
1	C	147[A]	VAL	2.7
1	F	74	ASP	2.7
1	C	225	ARG	2.5
1	D	125	ALA	2.5
1	E	97	ASP	2.4
1	C	80	GLU	2.4
1	F	202	GLU	2.4
1	E	126	GLY	2.4
1	C	202	GLU	2.3
1	F	208	ILE	2.3
1	E	177	PHE	2.2
1	F	108	PRO	2.2
1	E	225	ARG	2.2
1	F	201	GLU	2.1
1	B	153	ASP	2.1
1	E	85	LYS	2.0
1	E	63	GLU	2.0
1	B	198	PRO	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.