Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:54 AM GMT

PDB ID	:	3QBI
Title	:	Crystal structure of an anion-free yellow form of pharaonis halorhodopsin
Authors	:	Kouyama, T.; Kanada, S.
Deposited on	:	2011-01-13
Resolution	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

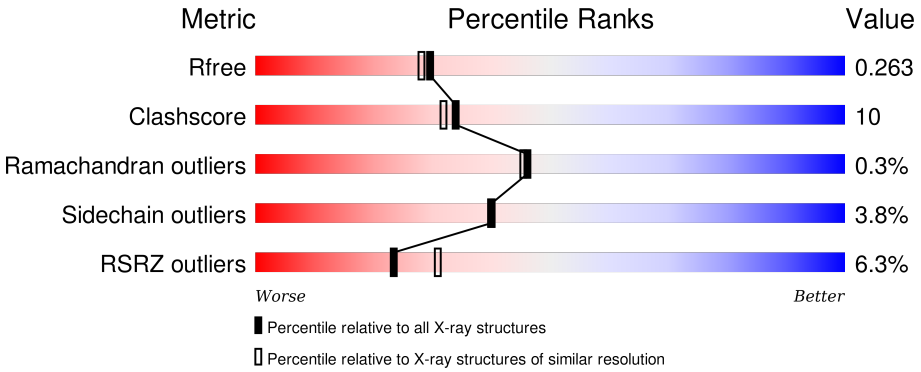
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 <=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	291	3%, 72%, 16%, 10%
1	B	291	8%, 68%, 21%, 11%
1	D	291	5%, 68%, 21%, 11%

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
2	RET	D	292	-	-	-	X
3	BNG	A	403	-	-	-	X
3	BNG	A	404	-	-	-	X
3	BNG	A	405	-	-	-	X
3	BNG	B	402	-	-	-	X
4	22B	B	300	-	-	-	X
4	22B	D	300	-	-	-	X

2 Entry composition

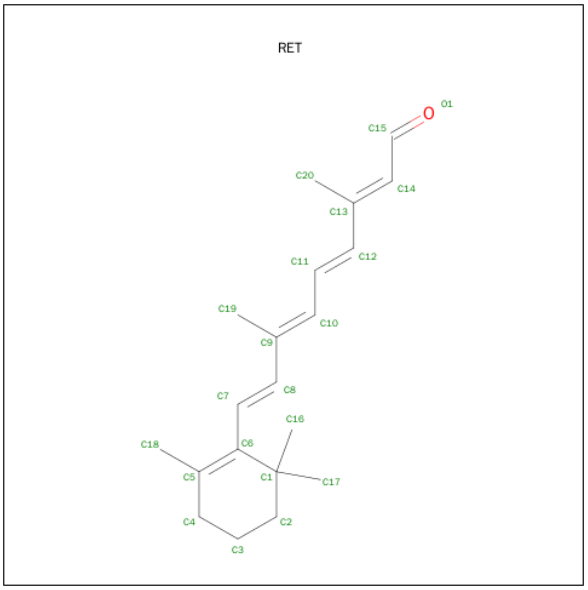
There are 5 unique types of molecules in this entry. The entry contains 6307 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Halorhodopsin.

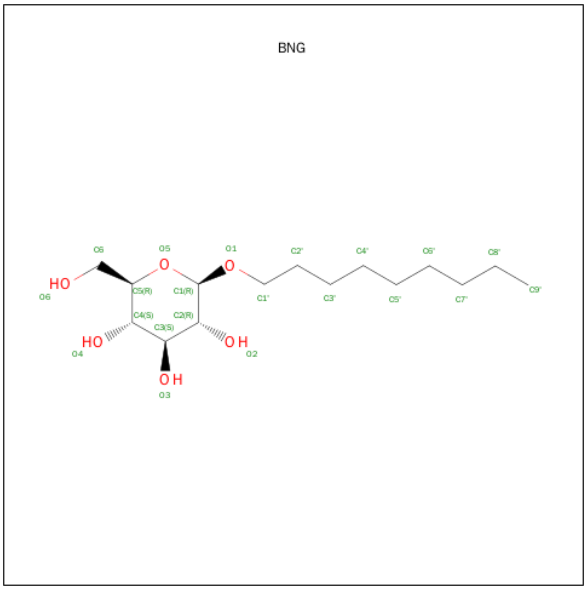
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			1971	1308	300	352	11			
1	B	260	Total	C	N	O	S	0	0	0
			1963	1302	299	351	11			
1	D	260	Total	C	N	O	S	0	0	0
			1963	1302	299	351	11			

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



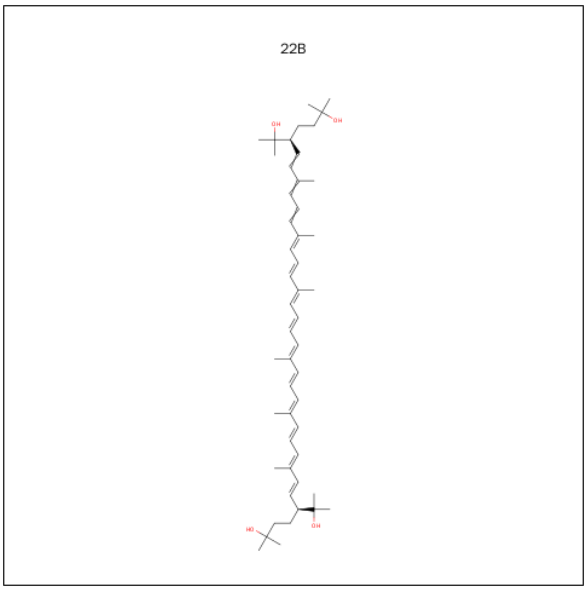
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		
2	B	1	Total	C	0	0
			20	20		
2	D	1	Total	C	0	0
			20	20		

- Molecule 3 is SUGAR (B-NONYLGLUCOSIDE) (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 21 15 6	0	0
3	A	1	Total C O 21 15 6	0	0
3	A	1	Total C O 21 15 6	0	0
3	B	1	Total C O 21 15 6	0	0

- Molecule 4 is BACTERIORUBERIN (three-letter code: 22B) (formula: $C_{50}H_{76}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 27 25 2	0	0
4	D	1	Total C O 27 25 2	0	0

- Molecule 5 is water.

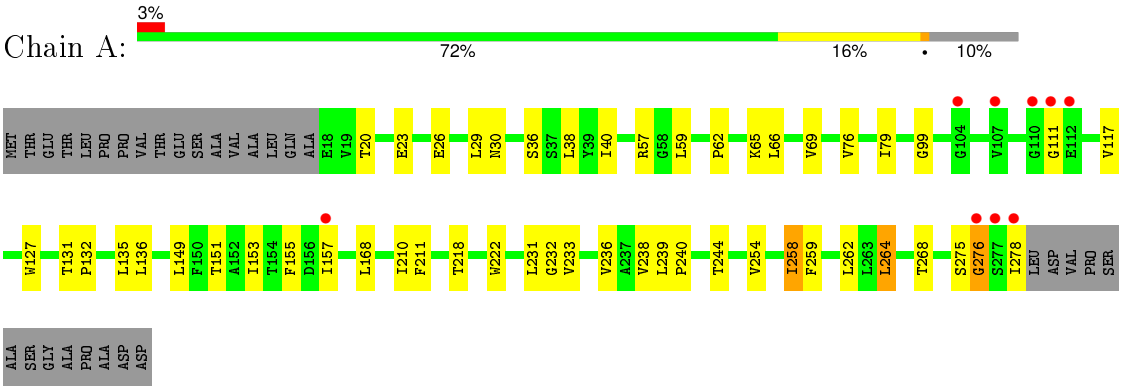
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	65	Total O 65 65	0	0
5	B	75	Total O 75 75	0	0
5	D	72	Total O 72 72	0	0

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.

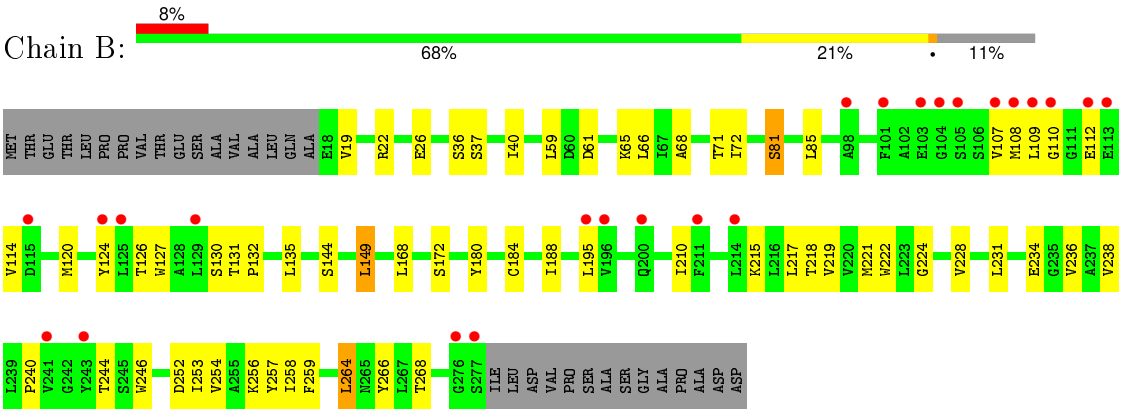
- Molecule 1: Halorhodopsin

Chain A:



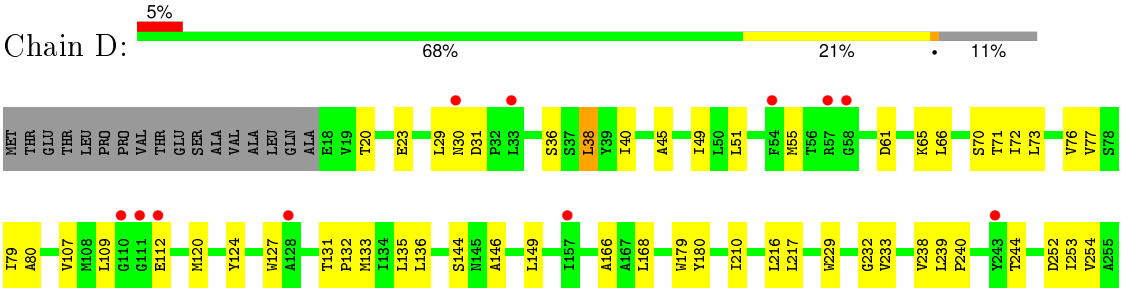
- Molecule 1: Halorhodopsin

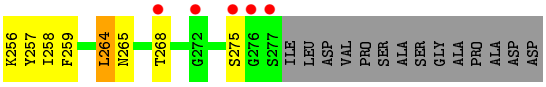
Chain B:



- Molecule 1: Halorhodopsin

Chain D:




K256
Y257
I258
F259
L264
N265
T268
G272
S275
G276
S277
ILE
LEU
ASP
VAL
PRO
SER
ALA
SER
GLY
ALA
PRO
ALA
ASP
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	153.96Å 97.97Å 100.65Å 90.00° 128.68° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10 42.39 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (15.00-2.10) 99.0 (42.39-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.10Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.235 , 0.266 0.232 , 0.263	Depositor DCC
R_{free} test set	3429 reflections (5.10%)	DCC
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 79.4	EDS
Estimated twinning fraction	0.018 for -h+k-l,-l,-k 0.008 for -h-k-l,l,k 0.040 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 67413 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6307	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BNG, 22B, RET

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	0.40	0/2017	0.58	0/2762
1	B	0.32	0/2009	0.54	0/2751
1	D	0.34	0/2009	0.54	0/2751
All	All	0.35	0/6035	0.55	0/8264

There are no bond length outliers.

There are no bond angle outliers.

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	1971	0	2025	32	0
1	B	1963	0	2014	48	0
1	D	1963	0	2014	45	0
2	A	20	0	27	1	0
2	B	20	0	27	4	0
2	D	20	0	27	3	0
3	A	63	0	90	1	0
3	B	21	0	30	0	0
4	B	27	0	37	3	0
4	D	27	0	37	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	65	0	0	1	0
5	B	75	0	0	8	0
5	D	72	0	0	4	0
All	All	6307	0	6328	126	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 10.

All (126) 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:233:VAL:H	1:A:244:THR:HG21	1.48	0.79
1:B:240:PRO:O	1:B:244:THR:HG23	1.83	0.77
1:A:240:PRO:O	1:A:244:THR:HG23	1.85	0.76
1:B:22:ARG:O	1:B:26:GLU:HG3	1.87	0.75
1:B:236:VAL:HG13	1:B:238:VAL:HG13	1.70	0.73
1:B:254:VAL:HG13	1:B:258:ILE:HD11	1.74	0.69
1:B:195:LEU:HD21	1:B:219:VAL:HG21	1.74	0.69
1:D:210:ILE:HA	5:D:600:HOH:O	1.93	0.68
1:B:108:MET:HA	1:B:112:GLU:O	1.94	0.68
1:A:264:LEU:O	1:A:268:THR:HG22	1.97	0.65
1:B:252:ASP:O	1:B:256:LYS:HB2	1.97	0.64
1:A:29:LEU:O	1:A:30:ASN:HB2	1.97	0.63
1:A:238:VAL:HG23	1:A:239:LEU:HD13	1.83	0.61
1:A:26:GLU:O	1:A:29:LEU:O	2.19	0.60
1:D:20:THR:OG1	1:D:23:GLU:HG3	2.01	0.60
1:D:233:VAL:H	1:D:244:THR:HG21	1.66	0.60
1:D:240:PRO:O	1:D:244:THR:HG23	2.01	0.60
1:D:238:VAL:HG23	1:D:239:LEU:HD13	1.82	0.59
1:A:236:VAL:HG13	1:A:238:VAL:HG13	1.85	0.59
1:D:107:VAL:HG22	1:D:109:LEU:HD13	1.84	0.58
1:D:73:LEU:HD13	1:D:133:MET:CE	2.34	0.58
1:B:258:ILE:HG13	1:B:259:PHE:N	2.18	0.58
1:B:81:SER:HB3	1:B:126:THR:OG1	2.03	0.58
1:B:109:LEU:HG	5:B:560:HOH:O	2.03	0.57
1:A:258:ILE:HG13	1:A:259:PHE:N	2.19	0.57
1:B:127:TRP:CD1	2:B:292:RET:H14	2.39	0.57
1:B:224:GLY:O	1:B:228:VAL:HG23	2.04	0.56
1:D:72:ILE:O	1:D:76:VAL:HG23	2.06	0.56
1:D:73:LEU:HD13	1:D:133:MET:HE3	1.88	0.56
1:A:254:VAL:HA	1:A:258:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLY:HA2	5:B:564:HOH:O	2.06	0.55
1:B:85:LEU:HD22	1:B:120:MET:HB3	1.89	0.55
1:B:184:CYS:O	1:B:188:ILE:HD13	2.07	0.55
1:B:195:LEU:HA	1:B:215:LYS:HD2	1.89	0.54
1:D:61:ASP:OD2	1:D:275:SER:HA	2.08	0.54
1:B:68:ALA:O	1:B:72:ILE:HG13	2.08	0.54
1:D:131:THR:OG1	1:D:132:PRO:HD3	2.08	0.54
1:D:252:ASP:O	1:D:256:LYS:HB2	2.08	0.53
1:B:19:VAL:HB	1:B:109:LEU:HD22	1.89	0.53
1:B:71:THR:HG21	1:B:264:LEU:HD13	1.92	0.52
1:D:232:GLY:HA2	1:D:244:THR:HG22	1.90	0.52
1:A:275:SER:O	1:A:276:GLY:C	2.48	0.52
1:D:45:ALA:O	1:D:49:ILE:HG13	2.10	0.51
1:B:81:SER:CB	1:B:126:THR:OG1	2.58	0.51
1:B:109:LEU:HD12	1:B:114:VAL:HB	1.93	0.51
1:A:127:TRP:CD1	2:A:292:RET:H14	2.46	0.51
1:D:254:VAL:HG13	1:D:258:ILE:HD11	1.93	0.51
1:A:218:THR:HG23	1:A:222:TRP:NE1	2.26	0.51
1:B:254:VAL:HA	1:B:258:ILE:HG12	1.92	0.50
1:B:231:LEU:O	1:B:238:VAL:HG22	2.12	0.50
1:A:29:LEU:O	1:A:30:ASN:CB	2.57	0.50
1:B:110:GLY:N	5:B:561:HOH:O	2.43	0.50
1:D:166:ALA:HB2	1:D:179:TRP:HB3	1.94	0.50
1:A:65:LYS:O	1:A:69:VAL:HG23	2.11	0.50
1:B:236:VAL:CG1	1:B:238:VAL:HG13	2.41	0.49
1:D:253:ILE:HA	1:D:257:TYR:CD2	2.48	0.49
1:D:61:ASP:O	1:D:65:LYS:HG3	2.13	0.49
1:D:71:THR:HG21	1:D:264:LEU:HD13	1.94	0.48
1:B:144:SER:OG	1:B:149:LEU:HD22	2.14	0.48
1:B:254:VAL:HG13	1:B:258:ILE:CD1	2.43	0.48
1:B:19:VAL:CG1	1:B:109:LEU:HD22	2.44	0.48
1:B:253:ILE:HA	1:B:257:TYR:CD2	2.48	0.48
1:D:264:LEU:O	1:D:268:THR:HG22	2.13	0.47
1:A:36:SER:O	1:A:40:ILE:HG12	2.15	0.47
1:B:131:THR:OG1	1:B:132:PRO:HD3	2.14	0.47
1:A:131:THR:N	1:A:132:PRO:CD	2.78	0.47
1:A:131:THR:OG1	1:A:132:PRO:HD3	2.15	0.46
1:D:73:LEU:O	1:D:77:VAL:HG23	2.15	0.46
1:A:231:LEU:O	1:A:238:VAL:HG22	2.15	0.46
1:D:258:ILE:HG13	1:D:259:PHE:N	2.29	0.46
1:D:127:TRP:CD1	2:D:292:RET:H14	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:VAL:HG23	1:A:239:LEU:CD1	2.45	0.46
1:B:268:THR:HG23	5:B:543:HOH:O	2.16	0.46
1:D:217:LEU:HD11	1:D:254:VAL:CG1	2.46	0.45
1:D:51:LEU:O	1:D:55:MET:HG3	2.16	0.45
1:D:70:SER:OG	1:D:136:LEU:HD12	2.16	0.45
1:D:232:GLY:CA	1:D:244:THR:HG22	2.46	0.45
1:A:151:THR:HG21	4:B:300:22B:H253	1.98	0.45
1:B:126:THR:O	1:B:130:SER:OG	2.30	0.45
1:A:258:ILE:O	1:A:262:LEU:HG	2.17	0.45
1:B:221:MET:SD	1:B:254:VAL:HG11	2.57	0.45
1:D:166:ALA:HB2	1:D:179:TRP:CB	2.46	0.45
1:B:61:ASP:O	1:B:65:LYS:HG3	2.18	0.45
1:D:136:LEU:HD13	1:D:136:LEU:C	2.38	0.44
1:B:124:TYR:HE2	2:B:292:RET:H162	1.83	0.44
1:B:210:ILE:HG21	1:B:266:TYR:CE2	2.53	0.44
1:B:218:THR:HG23	1:B:222:TRP:NE1	2.32	0.44
1:B:36:SER:O	1:B:40:ILE:HG12	2.17	0.44
1:B:217:LEU:O	1:B:221:MET:HG2	2.17	0.44
1:B:234:GLU:HG2	5:B:511:HOH:O	2.18	0.44
1:D:29:LEU:C	1:D:31:ASP:H	2.19	0.44
1:A:117:VAL:HG21	5:A:557:HOH:O	2.17	0.44
1:D:120:MET:HG2	5:D:509:HOH:O	2.17	0.44
1:B:109:LEU:HA	5:B:560:HOH:O	2.17	0.44
1:A:76:VAL:O	1:A:79:ILE:HG22	2.18	0.44
1:D:180:TYR:CD2	2:D:292:RET:H32	2.52	0.43
1:D:144:SER:HB3	1:D:149:LEU:CD2	2.48	0.43
1:A:254:VAL:O	1:A:258:ILE:HG13	2.18	0.43
1:A:232:GLY:HA2	1:A:239:LEU:HB2	2.00	0.43
1:B:195:LEU:CD2	1:B:219:VAL:HG21	2.45	0.42
1:D:254:VAL:HG13	1:D:258:ILE:CD1	2.48	0.42
1:D:238:VAL:HG23	1:D:239:LEU:CD1	2.47	0.42
1:D:216:LEU:C	1:D:216:LEU:HD13	2.40	0.42
1:D:265:ASN:ND2	5:D:543:HOH:O	2.53	0.42
1:A:153:ILE:O	1:A:157:ILE:HG13	2.19	0.42
1:A:62:PRO:HB2	1:A:278:ILE:HD11	2.02	0.42
1:A:278:ILE:HG21	1:D:146:ALA:HB3	2.01	0.42
1:A:155:PHE:CE1	4:B:300:22B:H192	2.55	0.42
1:D:38:LEU:HD21	1:D:120:MET:CE	2.50	0.42
5:B:607:HOH:O	1:D:65:LYS:HE2	2.20	0.41
1:B:210:ILE:HA	5:B:600:HOH:O	2.20	0.41
1:A:20:THR:OG1	1:A:23:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:TYR:HH	1:D:229:TRP:HE1	1.64	0.41
2:B:292:RET:H7	2:B:292:RET:H181	1.83	0.41
1:B:107:VAL:O	1:B:108:MET:HB3	2.20	0.41
1:D:36:SER:O	1:D:40:ILE:HG12	2.20	0.41
1:A:99:GLY:HA3	3:A:403:BNG:O2	2.20	0.41
1:B:180:TYR:CD2	2:B:292:RET:H32	2.55	0.41
1:B:72:ILE:HD12	4:B:300:22B:H163	2.02	0.41
1:D:79:ILE:HG23	1:D:80:ALA:N	2.35	0.41
2:D:292:RET:H7	2:D:292:RET:H181	1.84	0.41
1:B:37:SER:HB3	1:B:246:TRP:CD1	2.56	0.41
1:B:19:VAL:HG23	1:B:19:VAL:O	2.21	0.40
1:A:210:ILE:HG23	1:A:211:PHE:N	2.37	0.40
1:D:29:LEU:O	1:D:30:ASN:HB2	2.21	0.40
1:D:120:MET:HB2	5:D:506: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	259/291 (89%)	249 (96%)	8 (3%)	2 (1%)	24 17
1	B	258/291 (89%)	249 (96%)	9 (4%)	0	100 100
1	D	258/291 (89%)	252 (98%)	6 (2%)	0	100 100
All	All	775/873 (89%)	750 (97%)	23 (3%)	2 (0%)	46 45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	GLY
1	A	276	GLY

5.3.2 Protein sidechains (i)

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	209/233 (90%)	199 (95%)	10 (5%)	31	29
1	B	208/233 (89%)	200 (96%)	8 (4%)	40	40
1	D	208/233 (89%)	202 (97%)	6 (3%)	50	53
All	All	625/699 (89%)	601 (96%)	24 (4%)	40	40

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	57	ARG
1	A	59	LEU
1	A	66	LEU
1	A	135	LEU
1	A	136	LEU
1	A	149	LEU
1	A	168	LEU
1	A	258	ILE
1	A	264	LEU
1	B	59	LEU
1	B	66	LEU
1	B	81	SER
1	B	135	LEU
1	B	149	LEU
1	B	168	LEU
1	B	172	SER
1	B	264	LEU
1	D	38	LEU
1	D	66	LEU
1	D	112	GLU
1	D	135	LEU
1	D	168	LEU
1	D	264	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	B	41	ASN
1	B	265	ASN
1	B	270	ASN
1	D	265	ASN
1	D	270	ASN

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

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	RET	A	292	1	19,20,21	2.05	5 (26%)	27,27,28	1.52	6 (22%)
3	BNG	A	403	-	21,21,21	1.63	6 (28%)	26,26,26	0.70	0
3	BNG	A	404	-	21,21,21	1.64	5 (23%)	26,26,26	0.71	0
3	BNG	A	405	-	21,21,21	1.65	5 (23%)	26,26,26	0.72	0
2	RET	B	292	1	19,20,21	2.07	4 (21%)	27,27,28	1.72	8 (29%)
4	22B	B	300	-	24,26,53	3.57	9 (37%)	28,35,72	2.00	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BNG	B	402	-	21,21,21	1.64	6 (28%)	26,26,26	0.71	0
2	RET	D	292	1	19,20,21	2.02	4 (21%)	27,27,28	1.69	7 (25%)
4	22B	D	300	-	24,26,53	3.55	9 (37%)	28,35,72	2.01	9 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RET	A	292	1	-	0/13/30/31	0/1/1/1
3	BNG	A	403	-	-	0/12/32/32	0/1/1/1
3	BNG	A	404	-	-	0/12/32/32	0/1/1/1
3	BNG	A	405	-	-	0/12/32/32	0/1/1/1
2	RET	B	292	1	-	0/13/30/31	0/1/1/1
4	22B	B	300	-	-	0/31/31/65	0/0/0/0
3	BNG	B	402	-	-	0/12/32/32	0/1/1/1
2	RET	D	292	1	-	0/13/30/31	0/1/1/1
4	22B	D	300	-	-	0/31/31/65	0/0/0/0

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	292	RET	C2-C3	-2.47	1.45	1.52
2	B	292	RET	C2-C3	-2.43	1.45	1.52
2	D	292	RET	C2-C3	-2.41	1.46	1.52
3	B	402	BNG	C3-C2	2.03	1.57	1.52
3	A	403	BNG	C3-C2	2.03	1.57	1.52
2	A	292	RET	C2-C1	2.09	1.59	1.54
3	A	403	BNG	C1-C2	2.11	1.58	1.52
3	A	403	BNG	O5-C5	2.11	1.49	1.44
3	A	405	BNG	C1-C2	2.14	1.58	1.52
3	B	402	BNG	O5-C5	2.15	1.49	1.44
3	A	404	BNG	C1-C2	2.15	1.59	1.52
3	A	404	BNG	O5-C5	2.16	1.49	1.44
3	B	402	BNG	C1-C2	2.18	1.59	1.52
3	A	405	BNG	O5-C5	2.24	1.50	1.44
2	A	292	RET	C7-C6	2.55	1.55	1.45
4	D	300	22B	C18-C5	2.59	1.56	1.50
4	B	300	22B	C18-C5	2.60	1.56	1.50
3	A	403	BNG	C4-C5	2.61	1.58	1.53
2	B	292	RET	C7-C6	2.63	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	BNG	C4-C5	2.68	1.58	1.53
2	D	292	RET	C7-C6	2.71	1.55	1.45
3	A	405	BNG	C4-C5	2.78	1.59	1.53
3	B	402	BNG	C4-C5	2.89	1.59	1.53
4	B	300	22B	C20-C13	3.04	1.57	1.50
4	D	300	22B	C20-C13	3.05	1.57	1.50
4	B	300	22B	C17-C1	3.07	1.57	1.52
4	D	300	22B	C17-C1	3.28	1.58	1.52
4	B	300	22B	O27-C23	3.29	1.53	1.44
4	D	300	22B	O27-C23	3.45	1.54	1.44
3	B	402	BNG	O1-C1	3.68	1.46	1.40
4	D	300	22B	C16-C1	3.77	1.59	1.52
3	A	405	BNG	O1-C1	3.79	1.47	1.40
3	A	403	BNG	O1-C1	3.87	1.47	1.40
3	A	404	BNG	O1-C1	3.88	1.47	1.40
3	B	402	BNG	O5-C1	3.94	1.51	1.41
4	D	300	22B	C19-C9	3.95	1.59	1.50
3	A	403	BNG	O5-C1	3.95	1.52	1.41
4	B	300	22B	C19-C9	3.97	1.59	1.50
3	A	404	BNG	O5-C1	3.98	1.52	1.41
3	A	405	BNG	O5-C1	3.98	1.52	1.41
4	B	300	22B	C16-C1	4.01	1.59	1.52
4	B	300	22B	C22-C21	4.25	1.62	1.53
2	D	292	RET	C5-C6	4.32	1.41	1.34
2	B	292	RET	C5-C6	4.38	1.41	1.34
2	A	292	RET	C5-C6	4.40	1.41	1.34
4	D	300	22B	C22-C21	4.45	1.62	1.53
4	B	300	22B	C21-C2	4.88	1.60	1.54
4	D	300	22B	C21-C2	5.34	1.61	1.54
2	D	292	RET	C1-C6	5.80	1.62	1.53
2	A	292	RET	C1-C6	5.98	1.62	1.53
2	B	292	RET	C1-C6	6.19	1.62	1.53
4	D	300	22B	C2-C3	12.85	1.64	1.50
4	B	300	22B	C2-C3	13.19	1.64	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	300	22B	C17-C1-C16	-3.76	104.84	110.51
4	D	300	22B	C17-C1-C16	-3.54	105.19	110.51
4	D	300	22B	C4-C5-C6	-3.38	113.54	118.98
4	B	300	22B	C4-C5-C6	-3.33	113.62	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	292	RET	C1-C6-C5	-2.84	118.49	122.66
2	B	292	RET	C1-C6-C5	-2.79	118.57	122.66
2	A	292	RET	C1-C6-C5	-2.67	118.74	122.66
4	D	300	22B	C12-C13-C14	-2.61	110.44	118.92
4	B	300	22B	C12-C13-C14	-2.45	110.95	118.92
4	D	300	22B	C8-C9-C10	-2.37	115.16	118.98
2	D	292	RET	C8-C9-C10	-2.24	115.37	118.98
2	A	292	RET	C8-C9-C10	-2.13	115.55	118.98
4	B	300	22B	C8-C9-C10	-2.13	115.55	118.98
2	B	292	RET	C7-C6-C5	-2.08	116.60	121.37
2	B	292	RET	C2-C3-C4	2.01	116.60	111.53
2	B	292	RET	C19-C9-C8	2.04	121.49	118.10
2	A	292	RET	C2-C1-C6	2.04	113.60	110.36
2	A	292	RET	C17-C1-C6	2.24	113.82	110.30
2	D	292	RET	C2-C1-C6	2.26	113.94	110.36
4	D	300	22B	C24-C23-C22	2.40	118.70	111.59
2	D	292	RET	C19-C9-C8	2.40	122.09	118.10
2	B	292	RET	C20-C13-C12	2.43	122.14	118.10
4	B	300	22B	C24-C23-C22	2.43	118.81	111.59
2	D	292	RET	C20-C13-C12	2.57	122.37	118.10
2	D	292	RET	C17-C1-C6	2.60	114.38	110.30
2	B	292	RET	C2-C1-C6	2.64	114.55	110.36
2	A	292	RET	C20-C13-C12	2.65	122.51	118.10
4	B	300	22B	C18-C5-C4	2.74	122.66	118.10
4	D	300	22B	C18-C5-C4	2.75	122.68	118.10
2	B	292	RET	C17-C1-C6	2.76	114.63	110.30
2	A	292	RET	C1-C6-C7	2.85	123.80	115.82
2	D	292	RET	C1-C6-C7	3.13	124.57	115.82
2	B	292	RET	C1-C6-C7	3.22	124.83	115.82
4	D	300	22B	C16-C1-C2	3.55	116.95	111.59
4	B	300	22B	C20-C13-C12	3.88	124.56	118.10
4	B	300	22B	C16-C1-C2	3.98	117.61	111.59
4	D	300	22B	C20-C13-C12	4.13	124.97	118.10
4	B	300	22B	C21-C22-C23	4.23	124.85	116.36
4	D	300	22B	C21-C22-C23	4.28	124.97	116.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	292	RET	1	0
3	A	403	BNG	1	0
2	B	292	RET	4	0
4	B	300	22B	3	0
2	D	292	RET	3	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^{th} 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	261/291 (89%)	0.05	9 (3%) 49 58	15, 19, 38, 57	0
1	B	260/291 (89%)	0.52	24 (9%) 11 15	17, 32, 46, 63	0
1	D	260/291 (89%)	0.39	16 (6%) 24 32	17, 29, 44, 64	0
All	All	781/873 (89%)	0.32	49 (6%) 23 31	15, 27, 44, 64	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	277	SER	9.7
1	D	111	GLY	8.5
1	A	107	VAL	6.8
1	B	277	SER	6.5
1	D	276	GLY	6.5
1	B	276	GLY	6.2
1	B	243	TYR	5.3
1	B	109	LEU	4.9
1	D	110	GLY	4.9
1	B	110	GLY	4.2
1	B	104	GLY	4.0
1	D	30	ASN	4.0
1	B	241	VAL	4.0
1	B	98	ALA	3.9
1	A	277	SER	3.7
1	B	113	GLU	3.4
1	D	243	TYR	3.4
1	B	214	LEU	3.4
1	D	112	GLU	3.3
1	B	200	GLN	3.2
1	B	107	VAL	3.2
1	D	268	THR	3.1
1	A	276	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	110	GLY	3.0
1	B	195	LEU	3.0
1	D	57	ARG	3.0
1	D	275	SER	3.0
1	B	129	LEU	3.0
1	B	103	GLU	2.9
1	A	278	ILE	2.9
1	D	272	GLY	2.9
1	A	112	GLU	2.8
1	A	111	GLY	2.8
1	D	33	LEU	2.8
1	B	108	MET	2.7
1	B	105	SER	2.7
1	D	128	ALA	2.7
1	B	125	LEU	2.6
1	A	104	GLY	2.6
1	B	112	GLU	2.5
1	B	124	TYR	2.5
1	D	54	PHE	2.4
1	D	58	GLY	2.3
1	B	196	VAL	2.2
1	B	101	PHE	2.1
1	B	211	PHE	2.1
1	B	115	ASP	2.1
1	A	157	ILE	2.0
1	D	157	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^{th} 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
4	22B	D	300	27/54	0.66	0.35	6.66	74,77,84,84	0
4	22B	B	300	27/54	0.85	0.20	5.76	37,43,54,55	0
3	BNG	A	404	21/21	0.46	0.32	5.21	93,97,98,99	0
3	BNG	A	405	21/21	0.70	0.26	3.80	92,92,95,95	0
3	BNG	A	403	21/21	0.77	0.31	3.58	98,99,100,100	0
3	BNG	B	402	21/21	0.84	0.22	2.22	61,66,84,85	0
2	RET	D	292	20/21	0.86	0.17	2.03	20,24,32,32	0
2	RET	A	292	20/21	0.92	0.14	1.18	15,17,21,22	0
2	RET	B	292	20/21	0.91	0.12	-0.06	27,28,30,30	0

6.5 Other polymers

There are no such residues in this entry.