Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:53 PM GMT

PDB ID	:	4JRE
Title	:	Crystal structure of nitrate/nitrite exchanger NarK with nitrite bound
Authors	:	Zheng, H.; Wisedchaisri, G.; Gonen, T.
Deposited on	:	2013-03-21
Resolution	:	2.80 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:

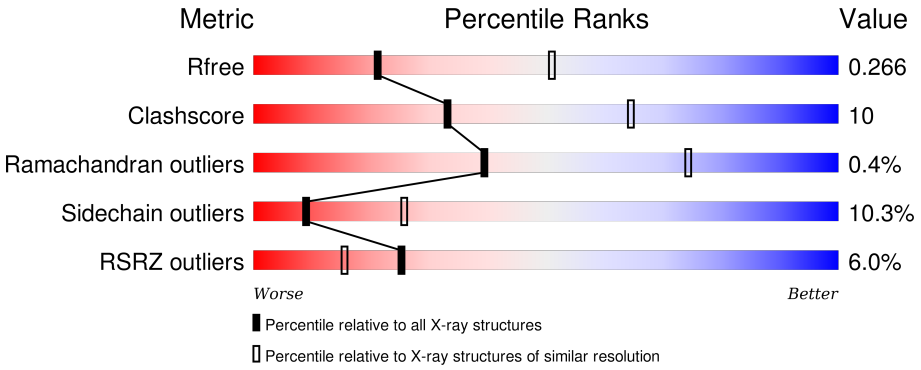
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	466	8% 67% 17% • 12%
1	D	466	12% 67% 17% • 14%
2	B	217	71% 22% 5% • •
2	H	217	69% 25% • • •
3	C	211	% 73% 22% •

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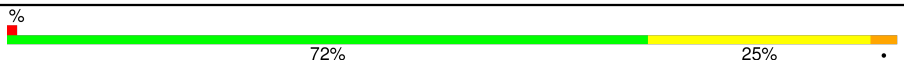
Mol	Chain	Length	Quality of chain
3	L	211	

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	NO2	D	501	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12589 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 Nitrite extrusion protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3088	2055	492	521	20			
1	D	402	Total	C	N	O	S	0	0	0
			3054	2040	484	510	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P10903
A	-1	SER	-	EXPRESSION TAG	UNP P10903
A	0	HIS	-	EXPRESSION TAG	UNP P10903
D	-2	GLY	-	EXPRESSION TAG	UNP P10903
D	-1	SER	-	EXPRESSION TAG	UNP P10903
D	0	HIS	-	EXPRESSION TAG	UNP P10903

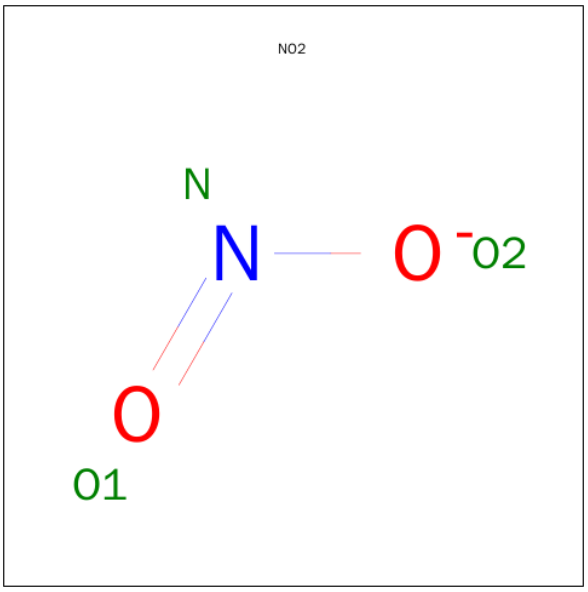
- Molecule 2 is a protein called Immunoglobulin Gamma-2a, Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1594	1017	261	309	7			
2	H	213	Total	C	N	O	S	0	0	0
			1592	1016	261	308	7			

- Molecule 3 is a protein called Immunoglobulin Kappa, Light chain.

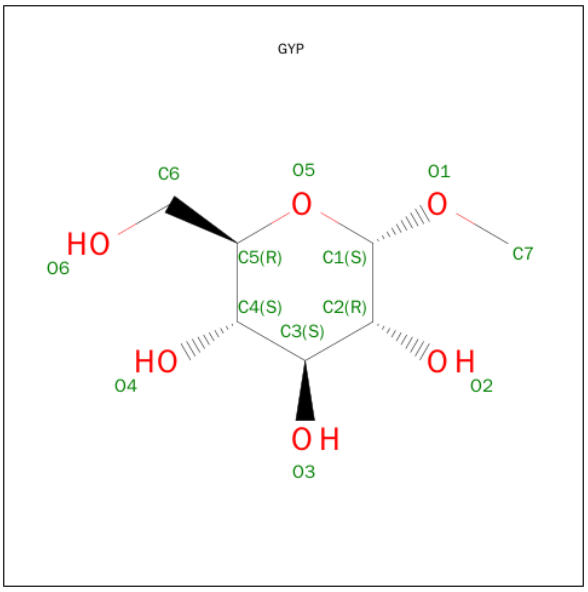
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	211	Total	C	N	O	S	0	0	0
			1597	1002	263	326	6			
3	L	211	Total	C	N	O	S	0	0	0
			1597	1002	262	327	6			

- Molecule 4 is NITRITE ION (three-letter code: NO2) (formula: NO_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N O 3 1 2	0	0
4	D	1	Total N O 3 1 2	0	0

- Molecule 5 is SUGAR (METHYL-ALPHA-D-GLUCOPYRANOSIDE) (three-letter code: GYP) (formula: $C_7H_{14}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 7 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 13 7 6	0	0

- Molecule 6 is water.

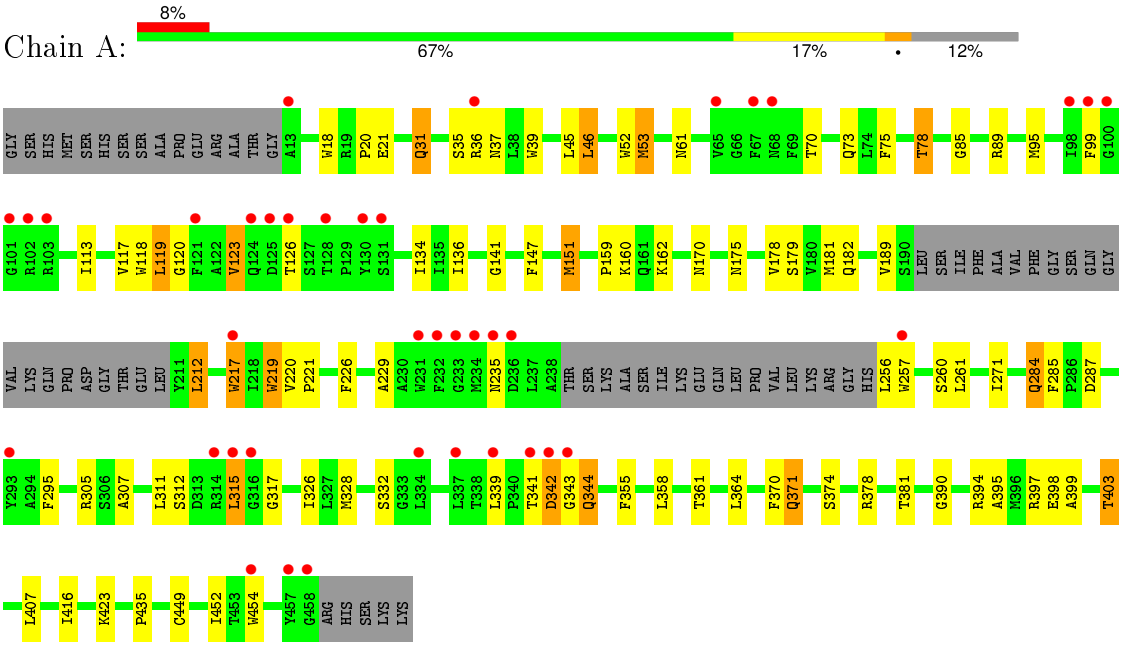
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	B	9	Total O 9 9	0	0
6	C	6	Total O 6 6	0	0
6	D	1	Total O 1 1	0	0
6	H	11	Total O 11 11	0	0
6	L	7	Total O 7 7	0	0

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.

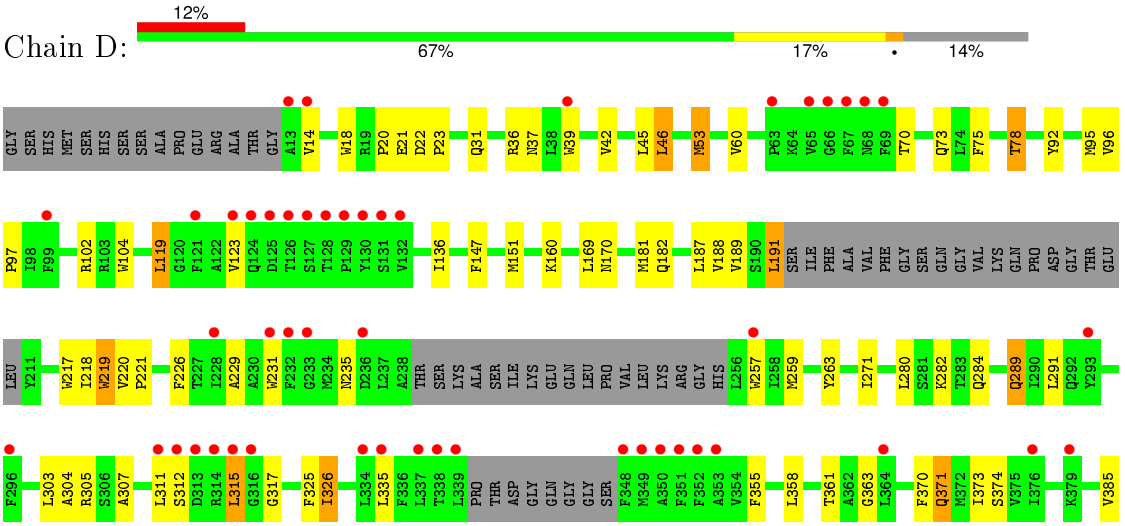
- Molecule 1: Nitrite extrusion protein 1

Chain A:



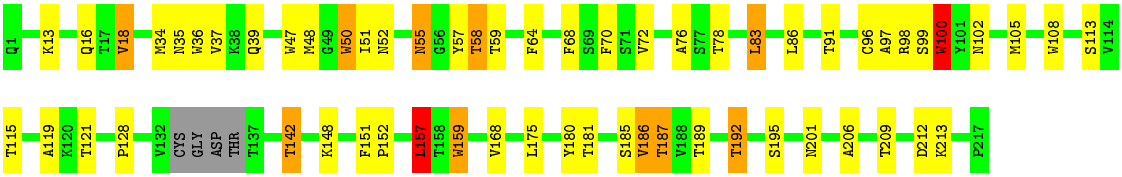
- Molecule 1: Nitrite extrusion protein 1

Chain D:



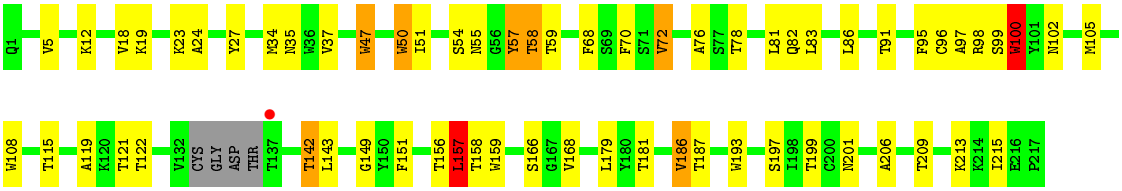
• Molecule 2: Immunoglobulin Gamma-2a, Heavy chain

Chain B:



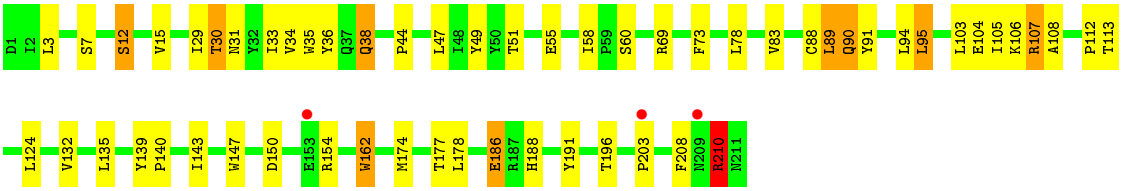
• Molecule 2: Immunoglobulin Gamma-2a, Heavy chain

Chain H:



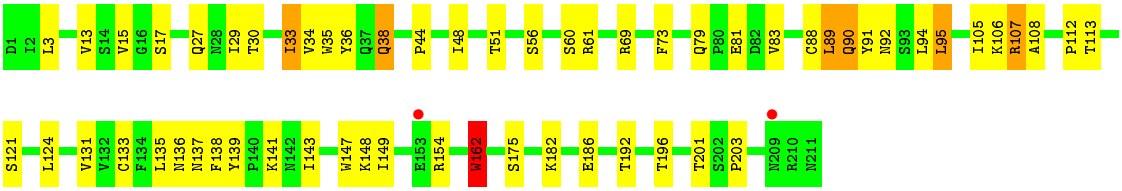
• Molecule 3: Immunoglobulin Kappa, Light chain

Chain C:



• Molecule 3: Immunoglobulin Kappa, Light chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.91Å 81.41Å 138.49Å 100.07° 96.38° 115.92°	Depositor
Resolution (Å)	50.00 – 2.80 47.04 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (50.00-2.80) 86.0 (47.04-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.223 , 0.269 0.223 , 0.266	Depositor DCC
R_{free} test set	3827 reflections (5.59%)	DCC
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.8	EDS
Estimated twinning fraction	0.001 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 72090 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12589	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: NO2, GYP

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	0.53	6/3173 (0.2%)	0.56	2/4312 (0.0%)
1	D	0.53	5/3138 (0.2%)	0.57	2/4263 (0.0%)
2	B	0.65	4/1638 (0.2%)	0.74	2/2237 (0.1%)
2	H	0.65	6/1636 (0.4%)	0.73	1/2234 (0.0%)
3	C	0.54	2/1633 (0.1%)	0.64	1/2230 (0.0%)
3	L	0.54	2/1633 (0.1%)	0.63	1/2230 (0.0%)
All	All	0.56	25/12851 (0.2%)	0.63	9/17506 (0.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	162	TRP	CD2-CE2	6.91	1.49	1.41
3	C	162	TRP	CD2-CE2	6.50	1.49	1.41
2	B	100	TRP	CD2-CE2	5.99	1.48	1.41
2	H	100	TRP	CD2-CE2	5.84	1.48	1.41
2	B	159	TRP	CD2-CE2	5.79	1.48	1.41
1	D	39	TRP	CD2-CE2	5.65	1.48	1.41
2	H	159	TRP	CD2-CE2	5.55	1.48	1.41
2	H	50	TRP	CD2-CE2	5.49	1.48	1.41
1	A	39	TRP	CD2-CE2	5.49	1.48	1.41
1	D	217	TRP	CD2-CE2	5.48	1.48	1.41
1	A	454	TRP	CD2-CE2	5.40	1.47	1.41
1	A	219	TRP	CD2-CE2	5.37	1.47	1.41
2	H	108	TRP	CD2-CE2	5.37	1.47	1.41
1	D	454	TRP	CD2-CE2	5.26	1.47	1.41
1	A	217	TRP	CD2-CE2	5.24	1.47	1.41
3	L	147	TRP	CD2-CE2	5.24	1.47	1.41
3	C	147	TRP	CD2-CE2	5.21	1.47	1.41
1	A	52	TRP	CD2-CE2	5.20	1.47	1.41
1	A	257	TRP	CD2-CE2	5.18	1.47	1.41
1	D	219	TRP	CD2-CE2	5.16	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	47	TRP	CD2-CE2	5.13	1.47	1.41
2	B	50	TRP	CD2-CE2	5.13	1.47	1.41
2	H	193	TRP	CD2-CE2	5.12	1.47	1.41
1	D	257	TRP	CD2-CE2	5.09	1.47	1.41
2	B	36	TRP	CD2-CE2	5.07	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	315	LEU	CA-CB-CG	6.06	129.23	115.30
2	B	157	LEU	CA-CB-CG	6.00	129.09	115.30
2	H	157	LEU	CA-CB-CG	5.75	128.53	115.30
1	D	46	LEU	CA-CB-CG	5.60	128.17	115.30
1	A	315	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	46	LEU	CA-CB-CG	5.37	127.66	115.30
3	L	95	LEU	CA-CB-CG	5.30	127.49	115.30
3	C	95	LEU	CA-CB-CG	5.24	127.35	115.30
2	B	100	TRP	CA-CB-CG	5.06	123.31	113.70

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	3088	0	3119	49	0
1	D	3054	0	3096	50	0
2	B	1594	0	1546	45	0
2	H	1592	0	1541	47	0
3	C	1597	0	1500	39	0
3	L	1597	0	1498	35	0
4	A	3	0	0	0	0
4	D	3	0	0	0	0
5	A	13	0	14	0	0
5	D	13	0	14	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	9	0	0	0	0
6	C	6	0	0	0	0
6	D	1	0	0	0	0
6	H	11	0	0	1	0
6	L	7	0	0	1	0
All	All	12589	0	12328	257	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 (257) 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:100:TRP:HE3	2:B:100:TRP:O	1.39	1.05
2:H:18:VAL:HG23	2:H:86:LEU:HD11	1.43	1.01
1:A:37:ASN:HD21	1:A:235:ASN:HD22	1.04	0.99
2:H:142:THR:HB	2:H:187:THR:HG22	1.47	0.96
2:H:35:ASN:HD22	2:H:47:TRP:HE1	1.13	0.96
2:H:50:TRP:CE2	2:H:100:TRP:HD1	1.84	0.94
1:A:36:ARG:NH2	1:A:235:ASN:HD21	1.64	0.94
2:H:37:VAL:HG21	2:H:105:MET:HE1	1.47	0.93
2:B:50:TRP:CE2	2:B:100:TRP:HD1	1.88	0.92
2:H:100:TRP:O	2:H:100:TRP:HE3	1.52	0.90
1:D:37:ASN:HD21	1:D:235:ASN:HD22	1.20	0.88
1:D:181:MET:HG3	1:D:219:TRP:HH2	1.39	0.86
2:B:37:VAL:CG2	2:B:105:MET:HE1	2.05	0.86
2:H:50:TRP:CE2	2:H:100:TRP:CD1	2.64	0.85
2:B:37:VAL:HG21	2:B:105:MET:HE1	1.56	0.84
2:H:37:VAL:CG2	2:H:105:MET:HE1	2.06	0.84
2:B:100:TRP:CE3	2:B:100:TRP:O	2.28	0.83
2:H:18:VAL:CG2	2:H:86:LEU:HD11	2.08	0.83
2:B:35:ASN:HD22	2:B:47:TRP:HE1	1.27	0.83
1:D:36:ARG:HH21	1:D:235:ASN:HD21	1.25	0.82
1:A:181:MET:HG3	1:A:219:TRP:CH2	2.14	0.81
2:B:34:MET:HE1	2:B:96:CYS:HB2	1.64	0.80
2:B:34:MET:CE	2:B:96:CYS:HB2	2.12	0.79
2:H:76:ALA:O	2:H:78:THR:HG23	1.82	0.79
2:H:50:TRP:CD2	2:H:100:TRP:HD1	2.02	0.78
1:A:399:ALA:O	1:A:403:THR:HG23	1.83	0.77
1:D:36:ARG:NH2	1:D:235:ASN:HD21	1.83	0.76
1:D:326:ILE:HD12	1:D:450:VAL:HG21	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:TRP:CE2	2:B:100:TRP:CD1	2.72	0.76
2:B:35:ASN:ND2	2:B:47:TRP:HE1	1.84	0.75
2:B:100:TRP:HZ3	3:C:91:TYR:O	1.70	0.75
1:A:36:ARG:HH21	1:A:235:ASN:HD21	1.33	0.75
2:H:100:TRP:O	2:H:100:TRP:CE3	2.39	0.75
2:H:142:THR:HB	2:H:187:THR:CG2	2.20	0.72
1:D:312:SER:OG	1:D:317:GLY:HA2	1.91	0.70
1:A:37:ASN:ND2	1:A:235:ASN:HD22	1.86	0.70
1:D:119:LEU:HB3	1:D:136:ILE:HG21	1.74	0.69
2:B:50:TRP:CD2	2:B:100:TRP:HD1	2.11	0.69
2:B:51:ILE:HD13	2:B:72:VAL:HG23	1.75	0.69
2:B:76:ALA:O	2:B:78:THR:HG23	1.93	0.68
1:A:119:LEU:HB3	1:A:136:ILE:HG21	1.76	0.68
1:D:181:MET:HG3	1:D:219:TRP:CH2	2.26	0.68
1:D:399:ALA:O	1:D:403:THR:HG23	1.94	0.66
3:L:148:LYS:HB2	3:L:192:THR:HB	1.78	0.66
3:C:196:THR:HG22	3:C:203:PRO:HB3	1.78	0.65
2:H:100:TRP:HZ3	3:L:91:TYR:O	1.79	0.65
2:B:100:TRP:CZ3	3:C:91:TYR:O	2.49	0.65
3:L:34:VAL:HG23	3:L:89:LEU:HB3	1.77	0.64
2:H:35:ASN:ND2	2:H:47:TRP:HE1	1.90	0.64
3:C:106:LYS:HE3	2:H:206:ALA:O	1.99	0.62
2:H:55:ASN:HB3	2:H:57:TYR:HB2	1.81	0.62
1:D:18:TRP:NE1	1:D:20:PRO:HG3	2.15	0.62
3:C:38:GLN:HG3	3:C:44:PRO:HG3	1.82	0.61
2:B:97:ALA:HB3	2:B:105:MET:HE2	1.82	0.61
2:B:58:THR:HG22	2:B:70:PHE:HB2	1.83	0.61
3:C:112:PRO:HG3	3:C:143:ILE:HD11	1.83	0.60
3:L:38:GLN:HG3	3:L:44:PRO:HG3	1.85	0.59
1:D:191:LEU:H	1:D:191:LEU:HD22	1.67	0.59
1:D:358:LEU:HA	1:D:361:THR:HG22	1.82	0.59
2:H:34:MET:CE	2:H:96:CYS:HB2	2.32	0.59
1:A:182:GLN:HE21	1:A:295:PHE:HA	1.66	0.59
2:B:37:VAL:HG23	2:B:105:MET:HE1	1.84	0.59
3:L:33:ILE:HG22	3:L:51:THR:HA	1.84	0.58
2:B:142:THR:HG22	2:B:187:THR:HB	1.84	0.58
2:H:98:ARG:O	2:H:105:MET:HA	2.03	0.58
3:L:35:TRP:CH2	3:L:88:CYS:HB3	2.38	0.58
1:A:358:LEU:HA	1:A:361:THR:HG22	1.85	0.58
3:L:162:TRP:N	3:L:162:TRP:CD1	2.72	0.58
1:A:123:VAL:HG21	1:A:212:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:ILE:HG21	3:C:90:GLN:HG3	1.87	0.57
2:H:143:LEU:HD22	2:H:215:ILE:HG21	1.86	0.57
2:B:18:VAL:HG22	2:B:86:LEU:HD11	1.85	0.57
1:D:53:MET:CE	1:D:53:MET:HA	2.34	0.56
2:H:168:VAL:HG22	2:H:186:VAL:CG1	2.35	0.56
1:D:21:GLU:OE2	1:D:160:LYS:HG2	2.05	0.56
1:A:307:ALA:O	1:A:311:LEU:HB2	2.05	0.56
1:D:188:VAL:HG21	1:D:218:ILE:HD12	1.88	0.56
1:A:18:TRP:NE1	1:A:20:PRO:HG3	2.21	0.56
3:L:34:VAL:HG13	3:L:91:TYR:CE1	2.41	0.56
2:H:91:THR:HG23	2:H:115:THR:HA	1.88	0.56
3:C:34:VAL:HG12	3:C:49:TYR:HA	1.88	0.56
1:D:181:MET:HE2	1:D:182:GLN:HG3	1.88	0.55
3:C:94:LEU:O	3:C:95:LEU:HD23	2.05	0.55
2:H:157:LEU:HD12	2:H:158:THR:N	2.22	0.55
2:H:100:TRP:CZ3	3:L:91:TYR:O	2.58	0.55
3:C:35:TRP:CZ3	3:C:88:CYS:HB3	2.42	0.55
2:H:50:TRP:CD2	2:H:100:TRP:CD1	2.89	0.55
2:H:34:MET:HE1	2:H:96:CYS:HB2	1.89	0.55
2:B:175:LEU:HB2	2:B:180:TYR:CE1	2.42	0.55
3:C:33:ILE:HG22	3:C:51:THR:HA	1.89	0.55
1:A:75:PHE:O	1:A:78:THR:HG22	2.07	0.54
3:L:196:THR:HG22	3:L:203:PRO:HB3	1.90	0.54
1:D:325:PHE:CE2	1:D:449:CYS:HB3	2.43	0.54
2:B:159:TRP:CE2	2:B:186:VAL:HG22	2.43	0.54
3:C:143:ILE:HG22	3:C:162:TRP:CZ3	2.43	0.54
3:C:35:TRP:CE2	3:C:73:PHE:HB2	2.43	0.54
3:C:35:TRP:CH2	3:C:88:CYS:HB3	2.43	0.53
3:L:107:ARG:HD2	3:L:139:TYR:CB	2.38	0.53
1:A:181:MET:CG	1:A:219:TRP:CH2	2.90	0.53
1:A:312:SER:OG	1:A:317:GLY:HA2	2.09	0.53
2:B:97:ALA:HB3	2:B:105:MET:CE	2.39	0.53
2:B:34:MET:HE1	2:B:96:CYS:CB	2.37	0.53
3:L:106:LYS:HA	3:L:139:TYR:OH	2.09	0.53
2:B:91:THR:HG23	2:B:115:THR:HA	1.90	0.52
3:C:34:VAL:HG13	3:C:91:TYR:CE1	2.44	0.52
2:B:157:LEU:HD12	2:B:157:LEU:C	2.30	0.52
3:L:143:ILE:HG22	3:L:162:TRP:CZ3	2.45	0.52
1:A:381:THR:HG21	1:A:398:GLU:HB2	1.92	0.52
1:D:147:PHE:O	1:D:151:MET:HB2	2.09	0.52
3:L:143:ILE:HG22	3:L:162:TRP:CH2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:SER:HG	1:D:317:GLY:HA2	1.75	0.52
2:H:50:TRP:CZ2	2:H:100:TRP:CD1	2.98	0.51
1:A:181:MET:CE	1:A:182:GLN:HG3	2.41	0.51
2:B:168:VAL:HG22	2:B:186:VAL:HG13	1.91	0.51
1:D:60:VAL:HG11	1:D:291:LEU:HD11	1.92	0.51
1:A:151:MET:HG2	1:A:407:LEU:HD21	1.92	0.51
3:C:12:SER:HB2	3:C:106:LYS:HE2	1.93	0.51
2:B:68:PHE:CE2	2:B:83:LEU:HD21	2.45	0.51
3:C:154:ARG:HG2	3:C:178:LEU:HD11	1.93	0.51
1:D:75:PHE:O	1:D:78:THR:HG22	2.11	0.51
1:D:325:PHE:CD2	1:D:449:CYS:HB3	2.47	0.50
3:C:12:SER:HA	3:C:104:GLU:O	2.11	0.50
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.46	0.50
1:A:449:CYS:HA	1:A:452:ILE:HG22	1.94	0.50
3:C:91:TYR:HA	3:C:95:LEU:HD22	1.93	0.50
1:A:312:SER:HB3	1:A:371:GLN:HG2	1.94	0.50
2:H:37:VAL:CG2	2:H:105:MET:CE	2.85	0.50
3:L:182:LYS:O	3:L:186:GLU:HB2	2.12	0.50
1:A:118:TRP:CE3	1:A:136:ILE:HG12	2.46	0.50
2:H:68:PHE:CE2	2:H:83:LEU:HD23	2.47	0.50
3:C:143:ILE:HG22	3:C:162:TRP:CH2	2.47	0.49
2:H:58:THR:HG22	2:H:70:PHE:HB2	1.94	0.49
1:D:373:ILE:HD13	1:D:410:ILE:HD13	1.94	0.49
3:L:112:PRO:HG3	3:L:143:ILE:HD11	1.93	0.49
3:C:186:GLU:O	3:C:210:ARG:NH2	2.45	0.49
3:L:107:ARG:HD3	3:L:108:ALA:O	2.12	0.49
1:D:263:TYR:OH	1:D:305:ARG:NH2	2.46	0.49
3:C:89:LEU:HD21	3:C:95:LEU:HD13	1.95	0.49
1:D:37:ASN:ND2	1:D:235:ASN:HD22	2.00	0.49
2:H:157:LEU:C	2:H:157:LEU:HD12	2.32	0.49
3:L:89:LEU:HD21	3:L:95:LEU:HD13	1.94	0.49
3:L:94:LEU:O	3:L:95:LEU:HD23	2.13	0.49
1:A:160:LYS:HG3	1:A:397:ARG:HG2	1.94	0.49
2:H:51:ILE:HD13	2:H:72:VAL:HG23	1.95	0.48
1:D:271:ILE:HG22	1:D:418:GLY:HA3	1.94	0.48
1:A:120:GLY:HA3	1:A:217:TRP:NE1	2.27	0.48
2:H:12:LYS:HG3	2:H:18:VAL:HG22	1.95	0.48
3:C:150:ASP:OD2	3:C:188:HIS:HB3	2.14	0.48
1:A:159:PRO:HG2	1:A:162:LYS:HB2	1.96	0.48
3:C:34:VAL:HG21	3:C:36:TYR:OH	2.13	0.48
2:H:55:ASN:HB3	2:H:57:TYR:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PHE:HA	1:A:229:ALA:HB3	1.94	0.48
2:B:13:LYS:HG3	2:B:16:GLN:NE2	2.29	0.47
2:B:119:ALA:HB3	2:B:151:PHE:CZ	2.50	0.47
1:A:31:GLN:O	1:A:35:SER:HB3	2.13	0.47
3:L:83:VAL:HG21	6:L:302:HOH:O	2.12	0.47
2:H:50:TRP:CZ2	2:H:100:TRP:HD1	2.28	0.47
3:C:107:ARG:HD3	3:C:108:ALA:O	2.15	0.47
1:A:175:ASN:ND2	1:A:305:ARG:HH11	2.12	0.47
1:D:181:MET:CG	1:D:219:TRP:HH2	2.20	0.47
2:B:128:PRO:HD3	2:B:213:LYS:HG2	1.96	0.47
1:D:70:THR:HB	1:D:73:GLN:H	1.79	0.47
3:C:34:VAL:CG2	3:C:89:LEU:HD23	2.44	0.47
1:D:449:CYS:HA	1:D:452:ILE:HG22	1.97	0.47
3:L:34:VAL:HG21	3:L:36:TYR:OH	2.15	0.47
2:H:37:VAL:HB	2:H:95:PHE:HB2	1.96	0.47
3:L:35:TRP:CE2	3:L:73:PHE:HB2	2.49	0.47
1:D:53:MET:HE3	1:D:53:MET:HA	1.97	0.47
2:H:97:ALA:HB3	2:H:105:MET:HE2	1.97	0.46
2:H:119:ALA:HB3	2:H:151:PHE:CE2	2.50	0.46
1:D:96:VAL:HB	1:D:97:PRO:HD3	1.98	0.46
1:A:45:LEU:HD23	1:A:170:ASN:O	2.15	0.46
1:A:371:GLN:HA	1:A:374:SER:HB3	1.96	0.46
3:C:47:LEU:HA	3:C:58:ILE:HG13	1.96	0.46
1:D:226:PHE:HA	1:D:229:ALA:HB3	1.98	0.46
2:B:48:MET:HG2	2:B:64:PHE:CE1	2.51	0.46
2:H:50:TRP:CD1	2:H:59:THR:HB	2.50	0.46
2:B:37:VAL:HG23	2:B:105:MET:CE	2.45	0.46
1:A:390:GLY:HA3	1:A:394:ARG:NH2	2.31	0.46
1:A:343:GLY:HA2	1:A:344:GLN:HA	1.69	0.46
1:A:381:THR:HG22	1:A:395:ALA:HA	1.98	0.46
2:B:52:ASN:HB3	2:B:55:ASN:OD1	2.16	0.46
3:L:91:TYR:CB	3:L:95:LEU:HD22	2.45	0.45
2:B:39:GLN:HE22	3:C:38:GLN:HE22	1.64	0.45
3:L:138:PHE:HE2	3:L:141:LYS:O	1.99	0.45
2:B:48:MET:HA	2:B:64:PHE:CD2	2.52	0.45
2:B:152:PRO:HD2	2:B:206:ALA:CB	2.46	0.45
2:B:212:ASP:O	2:B:213:LYS:HD2	2.17	0.45
2:H:142:THR:CB	2:H:187:THR:HG22	2.31	0.45
2:H:68:PHE:HE2	2:H:83:LEU:HD23	1.81	0.45
1:A:339:LEU:HD13	1:A:435:PRO:HG2	1.99	0.44
3:L:91:TYR:HA	3:L:95:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:TRP:CE2	3:L:95:LEU:HG	2.53	0.44
1:D:312:SER:HB3	1:D:371:GLN:HG2	1.99	0.44
3:C:55:GLU:HA	3:C:55:GLU:OE1	2.18	0.44
1:A:21:GLU:OE2	1:A:160:LYS:HG2	2.18	0.44
3:C:132:VAL:HG22	3:C:177:THR:HG22	2.00	0.44
2:B:50:TRP:CD1	2:B:59:THR:HB	2.53	0.44
1:A:378:ARG:HG3	1:A:399:ALA:HB1	1.98	0.44
2:H:149:GLY:HA2	2:H:179:LEU:HB3	1.99	0.44
2:B:34:MET:HE2	2:B:96:CYS:HB2	1.95	0.44
2:B:51:ILE:CD1	2:B:72:VAL:HG23	2.46	0.43
1:A:85:GLY:O	1:A:89:ARG:HG3	2.18	0.43
3:C:191:TYR:HB2	3:C:208:PHE:CE2	2.53	0.43
2:H:23:LYS:HA	2:H:78:THR:HG22	2.01	0.43
2:B:175:LEU:HD13	2:B:180:TYR:CE2	2.53	0.43
1:D:307:ALA:O	1:D:311:LEU:HB2	2.19	0.43
1:A:147:PHE:O	1:A:151:MET:HB2	2.19	0.43
3:C:94:LEU:C	3:C:95:LEU:HD23	2.39	0.43
3:L:34:VAL:HA	3:L:48:ILE:O	2.19	0.42
2:B:189:THR:OG1	2:B:192:THR:HG22	2.18	0.42
1:D:385:VAL:O	1:D:389:GLY:N	2.48	0.42
2:H:19:LYS:HA	2:H:81:LEU:O	2.19	0.42
1:D:102:ARG:HD2	1:D:231:TRP:O	2.19	0.42
3:C:33:ILE:CG2	3:C:51:THR:HA	2.50	0.42
1:D:335:LEU:HD23	1:D:439:MET:SD	2.59	0.42
1:A:220:VAL:N	1:A:221:PRO:HD2	2.35	0.42
2:H:70:PHE:HB3	6:H:303:HOH:O	2.19	0.42
1:D:435:PRO:O	1:D:439:MET:HB2	2.19	0.42
3:L:149:ILE:HD12	3:L:154:ARG:HD3	2.00	0.42
1:A:36:ARG:HH21	1:A:235:ASN:ND2	2.10	0.42
1:A:85:GLY:HA2	1:A:141:GLY:O	2.20	0.42
1:D:220:VAL:N	1:D:221:PRO:HD2	2.35	0.42
2:B:48:MET:HG2	2:B:64:PHE:CZ	2.54	0.42
1:A:341:THR:O	1:A:343:GLY:HA2	2.20	0.42
1:A:423:LYS:HD2	1:A:423:LYS:HA	1.86	0.42
1:D:280:LEU:C	1:D:282:LYS:H	2.23	0.42
3:L:34:VAL:CG2	3:L:89:LEU:HB3	2.46	0.42
1:D:304:ALA:HB3	1:D:363:GLY:HA3	2.02	0.42
3:L:89:LEU:HG	3:L:90:GLN:N	2.35	0.41
1:A:53:MET:HG2	1:A:178:VAL:HG13	2.02	0.41
1:A:284:GLN:HB3	1:A:285:PHE:CD1	2.55	0.41
1:D:259:MET:CE	1:D:259:MET:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:TYR:HA	1:D:95:MET:HG2	2.02	0.41
1:D:95:MET:HG3	1:D:104:TRP:CZ2	2.56	0.41
3:L:29:ILE:HG21	3:L:90:GLN:HG3	2.01	0.41
3:L:136:ASN:HB3	3:L:137:ASN:OD1	2.20	0.41
3:C:29:ILE:CG2	3:C:90:GLN:HG3	2.50	0.41
1:A:70:THR:HB	1:A:73:GLN:H	1.86	0.41
1:A:95:MET:HE3	1:A:99:PHE:HE2	1.85	0.41
1:D:271:ILE:HA	1:D:271:ILE:HD13	1.91	0.41
1:A:342:ASP:HA	1:A:343:GLY:HA3	1.94	0.41
3:C:139:TYR:CD1	3:C:140:PRO:HA	2.55	0.41
3:L:38:GLN:CG	3:L:44:PRO:HG3	2.50	0.41
1:D:456:VAL:HG12	1:D:456:VAL:O	2.21	0.41
1:D:289:GLN:HB3	1:D:289:GLN:HE21	1.75	0.41
3:L:13:VAL:CG1	3:L:17:SER:CB	2.99	0.41
1:D:45:LEU:HD11	1:D:147:PHE:HA	2.03	0.41
3:C:139:TYR:CG	3:C:140:PRO:HA	2.56	0.41
3:C:78:LEU:HD11	3:C:103:LEU:HD21	2.03	0.41
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.56	0.41
1:D:22:ASP:HA	1:D:23:PRO:HD2	1.94	0.40
1:A:61:ASN:CB	1:A:212:LEU:HD21	2.51	0.40
1:A:113:ILE:O	1:A:117:VAL:HG23	2.22	0.40
1:D:42:VAL:HG22	1:D:170:ASN:HA	2.04	0.40
2:B:108:TRP:CE2	3:C:44:PRO:HB2	2.57	0.40
3:C:30:THR:O	3:C:31:ASN:HB2	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	403/466 (86%)	384 (95%)	18 (4%)	1 (0%)	52 84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	394/466 (84%)	377 (96%)	17 (4%)	0	100	100
2	B	209/217 (96%)	197 (94%)	10 (5%)	2 (1%)	19	52
2	H	209/217 (96%)	200 (96%)	8 (4%)	1 (0%)	34	69
3	C	209/211 (99%)	193 (92%)	15 (7%)	1 (0%)	34	69
3	L	209/211 (99%)	197 (94%)	11 (5%)	1 (0%)	34	69
All	All	1633/1788 (91%)	1548 (95%)	79 (5%)	6 (0%)	39	74

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	SER
1	A	342	ASP
3	C	210	ARG
2	H	99	SER
3	L	92	ASN
2	B	55	ASN

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	314/364 (86%)	285 (91%)	29 (9%)	11	32
1	D	311/364 (85%)	288 (93%)	23 (7%)	17	43
2	B	175/182 (96%)	155 (89%)	20 (11%)	7	21
2	H	174/182 (96%)	153 (88%)	21 (12%)	6	18
3	C	178/190 (94%)	159 (89%)	19 (11%)	8	24
3	L	178/190 (94%)	153 (86%)	25 (14%)	4	13
All	All	1330/1472 (90%)	1193 (90%)	137 (10%)	9	26

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	46	LEU
1	A	53	MET
1	A	78	THR
1	A	119	LEU
1	A	123	VAL
1	A	126	THR
1	A	134	ILE
1	A	151	MET
1	A	179	SER
1	A	189	VAL
1	A	212	LEU
1	A	256	LEU
1	A	260	SER
1	A	261	LEU
1	A	271	ILE
1	A	284	GLN
1	A	287	ASP
1	A	315	LEU
1	A	326	ILE
1	A	328	MET
1	A	332	SER
1	A	344	GLN
1	A	355	PHE
1	A	364	LEU
1	A	370	PHE
1	A	371	GLN
1	A	403	THR
1	A	416	ILE
2	B	18	VAL
2	B	57	TYR
2	B	58	THR
2	B	83	LEU
2	B	98	ARG
2	B	100	TRP
2	B	102	ASN
2	B	113	SER
2	B	121	THR
2	B	142	THR
2	B	148	LYS
2	B	157	LEU
2	B	181	THR
2	B	185	SER

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Mol	Chain	Res	Type
2	B	186	VAL
2	B	187	THR
2	B	192	THR
2	B	195	SER
2	B	201	ASN
2	B	209	THR
3	C	3	LEU
3	C	7	SER
3	C	12	SER
3	C	15	VAL
3	C	30	THR
3	C	38	GLN
3	C	60	SER
3	C	69	ARG
3	C	83	VAL
3	C	89	LEU
3	C	90	GLN
3	C	105	ILE
3	C	107	ARG
3	C	113	THR
3	C	124	LEU
3	C	135	LEU
3	C	174	MET
3	C	186	GLU
3	C	210	ARG
1	D	14	VAL
1	D	31	GLN
1	D	46	LEU
1	D	53	MET
1	D	78	THR
1	D	119	LEU
1	D	123	VAL
1	D	169	LEU
1	D	187	LEU
1	D	189	VAL
1	D	191	LEU
1	D	284	GLN
1	D	289	GLN
1	D	303	LEU
1	D	315	LEU
1	D	326	ILE
1	D	355	PHE

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Mol	Chain	Res	Type
1	D	370	PHE
1	D	371	GLN
1	D	374	SER
1	D	403	THR
1	D	416	ILE
1	D	451	VAL
2	H	5	VAL
2	H	54	SER
2	H	57	TYR
2	H	58	THR
2	H	72	VAL
2	H	82	GLN
2	H	100	TRP
2	H	102	ASN
2	H	121	THR
2	H	122	THR
2	H	142	THR
2	H	156	THR
2	H	157	LEU
2	H	166	SER
2	H	181	THR
2	H	186	VAL
2	H	197	SER
2	H	199	THR
2	H	201	ASN
2	H	209	THR
2	H	213	LYS
3	L	3	LEU
3	L	15	VAL
3	L	27	GLN
3	L	30	THR
3	L	33	ILE
3	L	38	GLN
3	L	56	SER
3	L	60	SER
3	L	61	ARG
3	L	69	ARG
3	L	79	GLN
3	L	81	GLU
3	L	89	LEU
3	L	90	GLN
3	L	105	ILE

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Mol	Chain	Res	Type
3	L	107	ARG
3	L	113	THR
3	L	121	SER
3	L	124	LEU
3	L	131	VAL
3	L	133	CYS
3	L	135	LEU
3	L	162	TRP
3	L	175	SER
3	L	201	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	175	ASN
1	A	182	GLN
1	A	235	ASN
2	B	35	ASN
2	B	39	GLN
3	C	38	GLN
3	C	197	HIS
1	D	163	GLN
1	D	182	GLN
1	D	235	ASN
1	D	284	GLN
1	D	289	GLN
2	H	35	ASN
2	H	39	GLN
3	L	38	GLN
3	L	197	HIS

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
4	NO2	A	501	-	2,2,2	0.77	0	1,1,1	0.17	0
5	GYP	A	502	-	13,13,13	0.77	1 (7%)	18,18,18	1.46	2 (11%)
4	NO2	D	501	-	2,2,2	0.77	0	1,1,1	0.13	0
5	GYP	D	502	-	13,13,13	0.80	1 (7%)	18,18,18	1.44	2 (11%)

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
4	NO2	A	501	-	-	0/0/0/0	0/0/0/0
5	GYP	A	502	-	-	0/4/24/24	0/1/1/1
4	NO2	D	501	-	-	0/0/0/0	0/0/0/0
5	GYP	D	502	-	-	0/4/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	502	GYP	O1-C1	2.33	1.44	1.40
5	D	502	GYP	O1-C1	2.37	1.44	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	502	GYP	C1-O5-C5	2.63	118.84	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	502	GYP	C1-C2-C3	2.64	115.17	109.97
5	D	502	GYP	O1-C1-C2	4.50	113.52	108.21
5	A	502	GYP	O1-C1-C2	4.82	113.89	108.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	409/466 (87%)	0.24	39 (9%) 10 5	30, 73, 105, 139	0
1	D	402/466 (86%)	0.48	54 (13%) 4 2	30, 78, 105, 125	0
2	B	213/217 (98%)	-0.42	0 100 100	23, 36, 62, 112	0
2	H	213/217 (98%)	-0.49	1 (0%) 91 88	24, 35, 63, 94	0
3	C	211/211 (100%)	-0.33	3 (1%) 78 69	25, 41, 69, 84	0
3	L	211/211 (100%)	-0.31	2 (0%) 85 79	23, 40, 70, 84	0
All	All	1659/1788 (92%)	-0.03	99 (5%) 25 15	23, 53, 100, 139	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	126	THR	6.5
1	D	315	LEU	6.5
1	D	127	SER	6.4
1	D	431	LEU	6.0
1	A	65	VAL	5.8
1	D	13	ALA	5.3
1	A	343	GLY	5.2
1	D	314	ARG	5.1
1	D	131	SER	4.9
1	D	350	ALA	4.7
1	A	315	LEU	4.7
1	A	131	SER	4.7
1	D	349	MET	4.6
1	D	311	LEU	4.5
1	D	132	VAL	4.4
1	A	342	ASP	4.3
1	D	353	ALA	4.3
1	D	121	PHE	4.1
1	D	125	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	236	ASP	4.0
1	D	352	PHE	4.0
1	D	68	ASN	4.0
1	D	69	PHE	3.9
1	D	313	ASP	3.8
1	D	457	TYR	3.8
1	D	65	VAL	3.8
1	D	128	THR	3.8
1	A	67	PHE	3.7
1	A	99	PHE	3.7
1	D	67	PHE	3.7
1	A	68	ASN	3.7
1	D	124	GLN	3.7
1	A	128	THR	3.6
1	D	130	TYR	3.6
1	D	293	TYR	3.6
1	D	337	LEU	3.5
1	A	101	GLY	3.5
1	D	348	PHE	3.5
1	A	457	TYR	3.5
1	D	339	LEU	3.4
1	A	13	ALA	3.3
1	D	312	SER	3.3
1	A	316	GLY	3.3
1	A	124	GLN	3.2
1	D	257	TRP	3.2
1	A	235	ASN	3.2
1	D	296	PHE	3.1
1	D	231	TRP	3.1
1	A	341	THR	3.1
1	A	121	PHE	3.1
1	A	125	ASP	3.0
2	H	137	THR	3.0
1	A	314	ARG	3.0
1	A	102	ARG	3.0
1	A	130	TYR	3.0
1	D	99	PHE	2.9
3	C	209	ASN	2.9
1	D	232	PHE	2.9
1	A	98	ILE	2.9
1	A	454	TRP	2.8
1	A	339	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	456	VAL	2.8
1	A	236	ASP	2.8
1	A	231	TRP	2.7
1	A	458	GLY	2.7
1	D	233	GLY	2.7
1	D	14	VAL	2.7
1	A	126	THR	2.7
1	D	129	PRO	2.6
1	D	432	THR	2.5
1	A	36	ARG	2.5
1	D	376	ILE	2.4
1	A	100	GLY	2.4
1	D	334	LEU	2.4
1	A	337	LEU	2.4
1	D	66	GLY	2.4
1	D	123	VAL	2.3
3	L	153	GLU	2.3
1	A	257	TRP	2.3
1	A	232	PHE	2.3
1	D	351	PHE	2.3
3	C	153	GLU	2.3
1	D	338	THR	2.3
1	A	103	ARG	2.3
1	A	293	TYR	2.2
3	L	209	ASN	2.2
1	D	435	PRO	2.2
1	A	334	LEU	2.2
1	A	233	GLY	2.2
1	A	234	MET	2.1
1	D	228	ILE	2.1
1	D	335	LEU	2.1
1	D	316	GLY	2.1
1	D	379	LYS	2.1
1	A	217	TRP	2.1
3	C	203	PRO	2.1
1	D	39	TRP	2.0
1	D	364	LEU	2.0
1	D	63	PRO	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	NO2	D	501	3/3	0.91	0.31	5.46	71,71,72,73	0
5	GYP	A	502	13/13	0.86	0.19	1.53	82,91,99,106	0
4	NO2	A	501	3/3	0.76	0.19	1.24	78,78,80,80	0
5	GYP	D	502	13/13	0.86	0.18	-0.14	86,96,108,119	0

6.5 Other polymers (i)

There are no such residues in this entry.