Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:44 AM GMT

PDB ID	:	3BZU
Title	:	Crystal structure of human 11-beta-hydroxysteroid dehydrogenase(HSD1) in complex with NADP and thiazolone inhibitor
Authors	:	Min, X.; Sudom, A.; Xu, H.; Wang, Z.; Walker, N.P.
Deposited on	:	2008-01-18
Resolution	:	2.25 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:

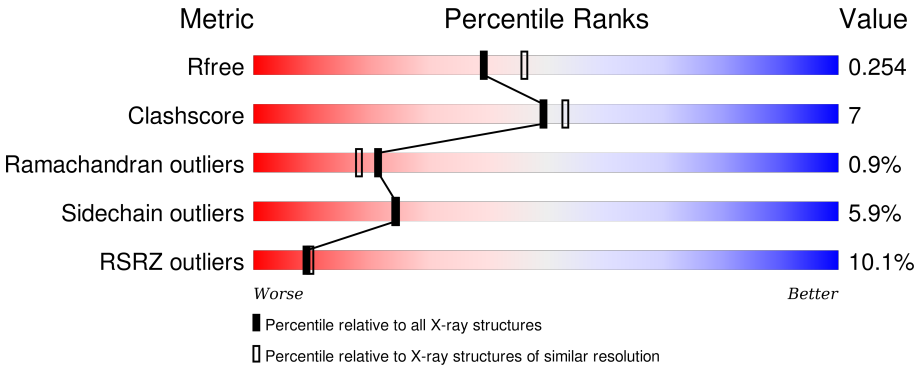
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	286	7% 74% 16% • 8%
1	B	286	7% 75% 15% • 8%
1	C	286	7% 72% 16% • 11%
1	D	286	15% 71% 15% •• 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8581 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	6	0
			2039	1299	341	383	16			
1	B	262	Total	C	N	O	S	0	3	0
			2011	1283	339	374	15			
1	C	254	Total	C	N	O	S	0	3	0
			1964	1254	330	365	15			
1	D	254	Total	C	N	O	S	0	1	0
			1946	1244	329	358	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	EXPRESSION TAG	UNP P28845
A	8	LYS	-	EXPRESSION TAG	UNP P28845
A	9	HIS	-	EXPRESSION TAG	UNP P28845
A	10	GLN	-	EXPRESSION TAG	UNP P28845
A	11	HIS	-	EXPRESSION TAG	UNP P28845
A	12	GLN	-	EXPRESSION TAG	UNP P28845
A	13	HIS	-	EXPRESSION TAG	UNP P28845
A	14	GLN	-	EXPRESSION TAG	UNP P28845
A	15	HIS	-	EXPRESSION TAG	UNP P28845
A	16	GLN	-	EXPRESSION TAG	UNP P28845
A	17	HIS	-	EXPRESSION TAG	UNP P28845
A	18	GLN	-	EXPRESSION TAG	UNP P28845
A	19	HIS	-	EXPRESSION TAG	UNP P28845
A	20	GLN	-	EXPRESSION TAG	UNP P28845
A	21	GLN	-	EXPRESSION TAG	UNP P28845
A	22	PRO	-	EXPRESSION TAG	UNP P28845
A	23	LEU	-	EXPRESSION TAG	UNP P28845
A	272	SER	CYS	ENGINEERED	UNP P28845
B	7	MET	-	EXPRESSION TAG	UNP P28845
B	8	LYS	-	EXPRESSION TAG	UNP P28845
B	9	HIS	-	EXPRESSION TAG	UNP P28845

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	EXPRESSION TAG	UNP P28845
B	11	HIS	-	EXPRESSION TAG	UNP P28845
B	12	GLN	-	EXPRESSION TAG	UNP P28845
B	13	HIS	-	EXPRESSION TAG	UNP P28845
B	14	GLN	-	EXPRESSION TAG	UNP P28845
B	15	HIS	-	EXPRESSION TAG	UNP P28845
B	16	GLN	-	EXPRESSION TAG	UNP P28845
B	17	HIS	-	EXPRESSION TAG	UNP P28845
B	18	GLN	-	EXPRESSION TAG	UNP P28845
B	19	HIS	-	EXPRESSION TAG	UNP P28845
B	20	GLN	-	EXPRESSION TAG	UNP P28845
B	21	GLN	-	EXPRESSION TAG	UNP P28845
B	22	PRO	-	EXPRESSION TAG	UNP P28845
B	23	LEU	-	EXPRESSION TAG	UNP P28845
B	272	SER	CYS	ENGINEERED	UNP P28845
C	7	MET	-	EXPRESSION TAG	UNP P28845
C	8	LYS	-	EXPRESSION TAG	UNP P28845
C	9	HIS	-	EXPRESSION TAG	UNP P28845
C	10	GLN	-	EXPRESSION TAG	UNP P28845
C	11	HIS	-	EXPRESSION TAG	UNP P28845
C	12	GLN	-	EXPRESSION TAG	UNP P28845
C	13	HIS	-	EXPRESSION TAG	UNP P28845
C	14	GLN	-	EXPRESSION TAG	UNP P28845
C	15	HIS	-	EXPRESSION TAG	UNP P28845
C	16	GLN	-	EXPRESSION TAG	UNP P28845
C	17	HIS	-	EXPRESSION TAG	UNP P28845
C	18	GLN	-	EXPRESSION TAG	UNP P28845
C	19	HIS	-	EXPRESSION TAG	UNP P28845
C	20	GLN	-	EXPRESSION TAG	UNP P28845
C	21	GLN	-	EXPRESSION TAG	UNP P28845
C	22	PRO	-	EXPRESSION TAG	UNP P28845
C	23	LEU	-	EXPRESSION TAG	UNP P28845
C	272	SER	CYS	ENGINEERED	UNP P28845
D	7	MET	-	EXPRESSION TAG	UNP P28845
D	8	LYS	-	EXPRESSION TAG	UNP P28845
D	9	HIS	-	EXPRESSION TAG	UNP P28845
D	10	GLN	-	EXPRESSION TAG	UNP P28845
D	11	HIS	-	EXPRESSION TAG	UNP P28845
D	12	GLN	-	EXPRESSION TAG	UNP P28845
D	13	HIS	-	EXPRESSION TAG	UNP P28845
D	14	GLN	-	EXPRESSION TAG	UNP P28845
D	15	HIS	-	EXPRESSION TAG	UNP P28845

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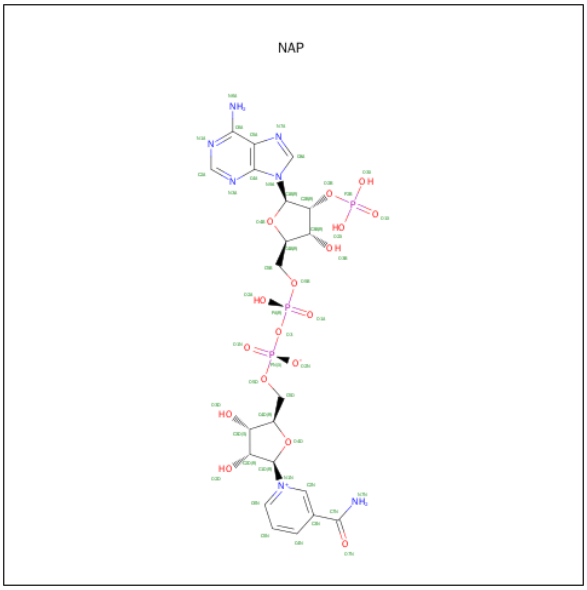
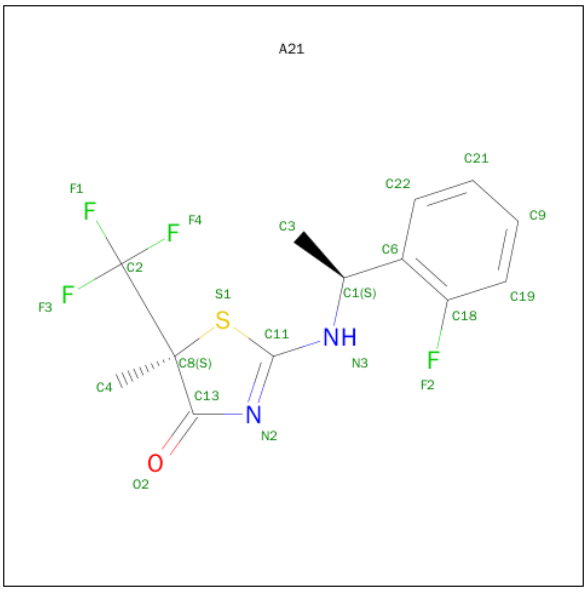
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	EXPRESSION TAG	UNP P28845
D	17	HIS	-	EXPRESSION TAG	UNP P28845
D	18	GLN	-	EXPRESSION TAG	UNP P28845
D	19	HIS	-	EXPRESSION TAG	UNP P28845
D	20	GLN	-	EXPRESSION TAG	UNP P28845
D	21	GLN	-	EXPRESSION TAG	UNP P28845
D	22	PRO	-	EXPRESSION TAG	UNP P28845
D	23	LEU	-	EXPRESSION TAG	UNP P28845
D	272	SER	CYS	ENGINEERED	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 3 is (5S)-2-{[(1S)-1-(2-FLUOROPHENYL)ETHYL]AMINO}-5-METHYL-5-(TRIFLUOROMETHYL)-1,3-THIAZOL-4(5H)-ONE (three-letter code: A21) (formula: $C_{13}H_{12}F_4N_2OS$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N O S 21 13 4 2 1 1	0	0
3	B	1	Total C F N O S 21 13 4 2 1 1	0	0
3	C	1	Total C F N O S 21 13 4 2 1 1	0	0
3	D	1	Total C F N O S 21 13 4 2 1 1	0	0

- Molecule 4 is water.

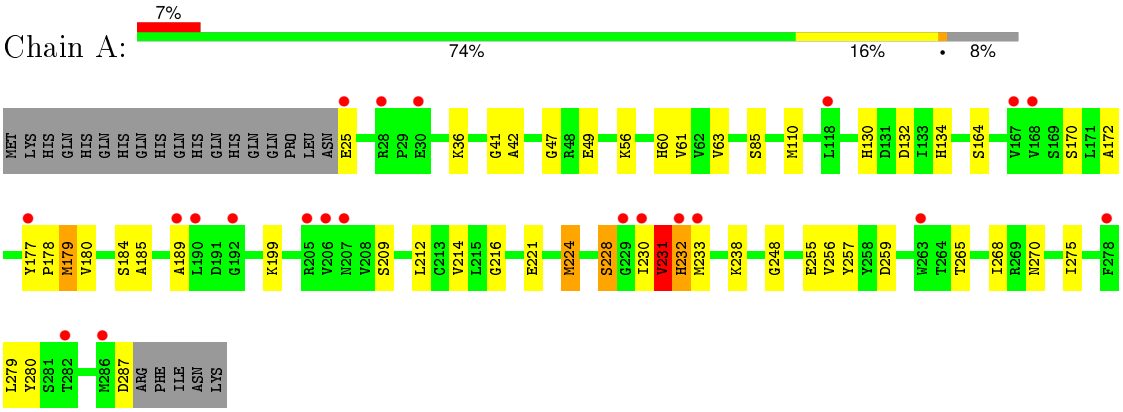
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	104	Total O 104 104	0	0
4	B	99	Total O 99 99	0	0
4	C	97	Total O 97 97	0	0
4	D	45	Total O 45 45	0	0

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.

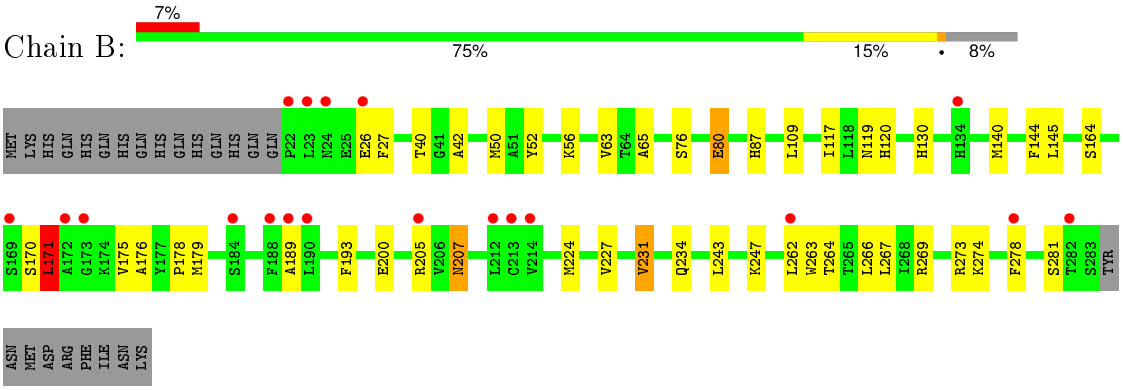
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain A:



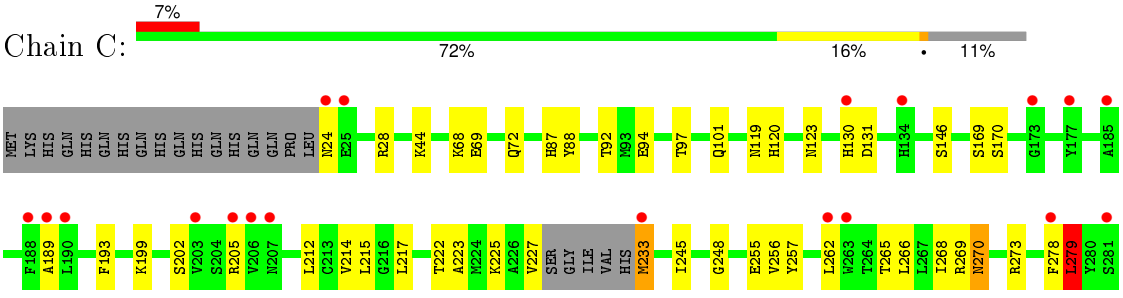
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain B:



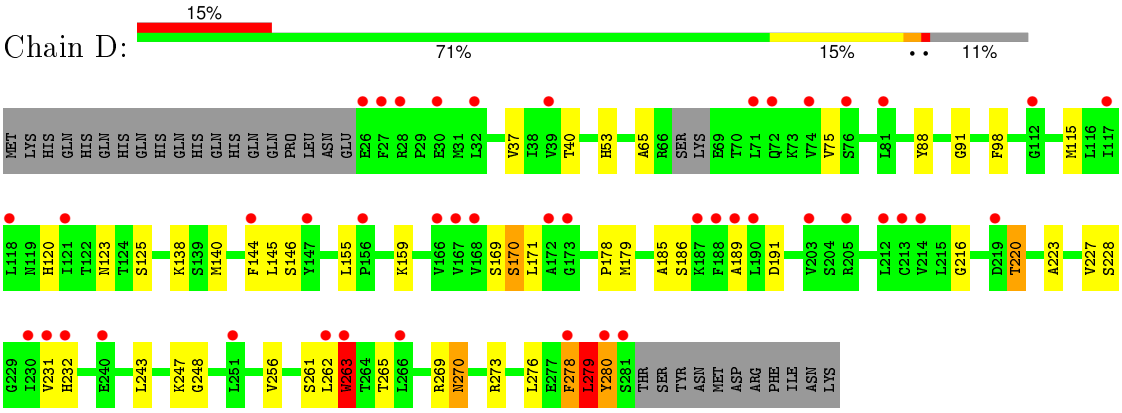
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain C:



• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.02Å 153.01Å 73.72Å 90.00° 92.16° 90.00°	Depositor
Resolution (Å)	31.33 – 2.25 36.84 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.5 (31.33-2.25) 96.5 (36.84-2.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.3.0026	Depositor
R, R_{free}	0.201 , 0.263 0.196 , 0.254	Depositor DCC
R_{free} test set	2862 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.3	EDS
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 56602 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8581	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: A21, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.65	0/2099	0.67	0/2835
1	B	0.64	0/2058	0.71	2/2779 (0.1%)
1	C	0.62	0/2008	0.65	0/2710
1	D	0.56	0/1982	0.67	1/2675 (0.0%)
All	All	0.62	0/8147	0.68	3/10999 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	279	LEU	CA-CB-CG	8.35	134.50	115.30
1	B	171	LEU	CA-CB-CG	6.05	129.22	115.30
1	B	273	ARG	NE-CZ-NH2	-5.86	117.37	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	D	278	PHE	Peptide

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	2039	0	2069	30	0
1	B	2011	0	2063	33	0
1	C	1964	0	2006	26	0
1	D	1946	0	1992	37	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
3	A	21	0	12	0	0
3	B	21	0	12	0	0
3	C	21	0	12	0	0
3	D	21	0	12	0	0
4	A	104	0	0	2	0
4	B	99	0	0	7	0
4	C	97	0	0	4	0
4	D	45	0	0	1	0
All	All	8581	0	8278	117	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 7.

All (117) 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:B:227:VAL:HB	1:B:231:VAL:CG1	1.90	1.02
1:A:224:MET:HA	1:A:224:MET:HE3	1.48	0.92
1:D:243:LEU:O	1:D:247:LYS:HG3	1.81	0.79
1:A:178:PRO:O	1:A:179:MET:HB2	1.83	0.78
1:B:227:VAL:HB	1:B:231:VAL:HG12	1.64	0.77
1:C:130:HIS:HB3	4:C:477:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:HIS:HB3	4:B:358:HOH:O	1.87	0.73
1:B:274:LYS:O	1:B:278:PHE:CD1	2.42	0.73
1:D:140:MET:HE2	1:D:144:PHE:HB3	1.72	0.71
1:C:92:THR:OG1	1:C:94:GLU:HG3	1.91	0.70
1:C:72[B]:GLN:HG2	1:C:88:TYR:CE2	2.27	0.70
1:B:140:MET:HA	1:B:140:MET:HE3	1.76	0.67
1:A:224:MET:HA	1:A:224:MET:CE	2.23	0.66
1:D:276:LEU:O	1:D:279:LEU:HD13	1.96	0.66
1:A:275:ILE:HD12	1:C:266:LEU:HD12	1.77	0.65
1:D:140:MET:CE	1:D:144:PHE:HB3	2.27	0.65
1:D:220:THR:HG22	1:D:223:ALA:H	1.63	0.63
1:D:220:THR:HG21	2:D:4:NAP:O2N	1.99	0.62
1:D:140:MET:CE	1:D:186:SER:HA	2.31	0.61
1:A:216:GLY:HA3	1:A:259:ASP:OD2	2.01	0.60
1:D:37:VAL:HG13	1:D:115:MET:HB3	1.82	0.60
1:A:164:SER:HB2	4:A:352:HOH:O	2.02	0.60
1:C:120:HIS:HE1	1:C:146:SER:OG	1.85	0.59
1:D:140:MET:HE3	1:D:186:SER:HA	1.84	0.59
1:A:231:VAL:O	1:A:232:HIS:HB2	2.02	0.59
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.85	0.58
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.86	0.58
1:D:270:ASN:HD22	1:D:270:ASN:C	2.07	0.58
1:C:270:ASN:ND2	1:C:273:ARG:H	2.02	0.58
1:B:87:HIS:HD2	4:B:384:HOH:O	1.87	0.57
1:B:243:LEU:HG	1:B:247:LYS:HE3	1.87	0.57
1:A:172:ALA:HB2	1:A:177[A]:TYR:HD2	1.70	0.56
1:B:42:ALA:HB3	1:B:63:VAL:HB	1.88	0.55
1:B:140:MET:HE3	1:B:144:PHE:HB3	1.88	0.55
1:A:60:HIS:HD2	1:A:85:SER:OG	1.89	0.55
1:D:278:PHE:C	1:D:280:TYR:H	2.09	0.54
1:D:140:MET:CE	1:D:144:PHE:CB	2.86	0.54
1:D:279:LEU:O	1:D:279:LEU:HD22	2.08	0.54
1:C:270:ASN:C	1:C:270:ASN:HD22	2.11	0.54
1:C:120:HIS:CE1	1:C:146:SER:OG	2.61	0.54
1:D:263:TRP:HE3	1:D:263:TRP:C	2.11	0.53
1:A:199:LYS:HE2	1:B:176:ALA:HB3	1.91	0.53
1:C:97:THR:HG22	1:C:101:GLN:NE2	2.23	0.53
1:D:178:PRO:O	1:D:179:MET:HB2	2.09	0.53
1:B:227:VAL:HB	1:B:231:VAL:HG13	1.84	0.52
1:A:224:MET:O	1:A:228:SER:HB2	2.09	0.52
1:D:223:ALA:O	1:D:227:VAL:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:HD22	1:B:175:VAL:HG22	1.92	0.52
1:A:164:SER:HB3	1:A:209:SER:OG	2.10	0.52
1:B:205:ARG:NH1	4:B:380:HOH:O	2.42	0.52
1:B:27:PHE:CD2	1:B:247:LYS:HG2	2.46	0.51
1:C:193:PHE:HB2	1:D:185:ALA:HB2	1.92	0.51
1:A:170:SER:O	1:A:214:VAL:HG13	2.11	0.51
1:A:280:TYR:OH	1:B:264:THR:HG21	2.11	0.51
1:A:257:TYR:CD2	1:A:268:ILE:HG23	2.46	0.51
1:B:26:GLU:HG2	4:B:364:HOH:O	2.10	0.50
1:B:262:LEU:HG	4:B:349:HOH:O	2.11	0.50
1:C:257:TYR:CE1	1:C:269:ARG:HG2	2.47	0.49
1:D:276:LEU:O	1:D:279:LEU:CD1	2.60	0.49
1:D:53:HIS:CE1	1:D:243:LEU:HD22	2.47	0.49
1:B:263:TRP:HA	1:B:266:LEU:HD13	1.93	0.49
1:B:224:MET:HA	1:B:224:MET:CE	2.42	0.49
1:C:87:HIS:HD2	4:C:394:HOH:O	1.95	0.49
1:C:214:VAL:HG11	1:C:268:ILE:HG12	1.95	0.49
1:A:132[A]:ASP:OD1	1:A:134:HIS:CE1	2.66	0.48
1:C:223:ALA:O	1:C:227:VAL:HG22	2.13	0.48
1:D:248:GLY:HA3	1:D:256:VAL:HG21	1.96	0.48
1:B:52:TYR:O	1:B:56:LYS:HG3	2.14	0.47
1:A:275:ILE:CD1	1:C:266:LEU:HD12	2.42	0.47
1:D:261:SER:OG	1:D:263:TRP:HB3	2.14	0.47
1:B:76:SER:O	1:B:80:GLU:HG2	2.14	0.47
1:B:178:PRO:O	1:B:179:MET:HB2	2.14	0.47
1:A:132[A]:ASP:OD1	1:A:134:HIS:NE2	2.48	0.46
1:A:36:LYS:HE2	1:A:110:MET:O	2.16	0.46
1:D:120:HIS:HE1	1:D:146:SER:OG	1.99	0.46
1:D:155:LEU:HG	1:D:159:LYS:HE3	1.98	0.46
1:C:279:LEU:HD11	1:D:263:TRP:CH2	2.50	0.46
1:A:185:ALA:HB2	1:B:193:PHE:HB2	1.97	0.45
1:D:140:MET:HE2	1:D:144:PHE:CB	2.45	0.45
1:A:60:HIS:CD2	1:A:85:SER:OG	2.68	0.45
1:B:278:PHE:O	1:B:281:SER:HB3	2.17	0.45
1:A:180:VAL:O	1:A:184[A]:SER:OG	2.30	0.45
1:D:170:SER:HB3	2:D:4:NAP:H5N	1.98	0.44
1:C:217:LEU:HD22	1:C:233:MET:HB2	1.99	0.44
1:B:164:SER:HB3	4:B:310:HOH:O	2.18	0.44
1:D:191:ASP:HB2	4:D:306:HOH:O	2.18	0.44
1:B:263:TRP:HA	1:B:266:LEU:CD1	2.47	0.44
1:A:49:GLU:HG3	1:A:238:LYS:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ALA:O	1:A:184[B]:SER:HB2	2.18	0.43
1:B:50:MET:CE	1:B:117:ILE:HG21	2.48	0.43
1:A:56:LYS:NZ	4:A:366:HOH:O	2.42	0.43
1:D:270:ASN:C	1:D:270:ASN:ND2	2.70	0.43
1:D:75:VAL:HG21	1:D:88:TYR:HB3	2.00	0.43
1:C:68:LYS:NZ	4:C:463:HOH:O	2.52	0.42
1:C:169:SER:OG	1:C:170:SER:N	2.51	0.42
1:B:170:SER:OG	2:B:2:NAP:H6N	2.20	0.42
1:D:171:LEU:HG	1:D:216:GLY:HA2	2.01	0.42
1:B:40:THR:OG1	1:B:120:HIS:HD2	2.03	0.42
1:C:123:ASN:N	1:C:123:ASN:HD22	2.18	0.42
1:A:41:GLY:O	1:A:47:GLY:HA3	2.19	0.42
1:D:263:TRP:CE3	1:D:263:TRP:C	2.92	0.42
1:C:215:LEU:HD11	1:C:245:ILE:HD11	2.01	0.41
1:D:270:ASN:ND2	1:D:273:ARG:H	2.18	0.41
1:D:227:VAL:HB	1:D:231:VAL:HG22	2.01	0.41
1:D:91:GLY:HA3	1:D:98:PHE:CZ	2.55	0.41
1:A:189:ALA:HB2	1:B:189:ALA:HB2	2.01	0.41
1:A:248:GLY:HA3	1:A:256:VAL:CG2	2.50	0.41
1:D:169:SER:OG	1:D:170:SER:N	2.53	0.41
1:C:212:LEU:O	1:C:255:GLU:HA	2.20	0.41
1:C:119:ASN:OD1	2:C:3:NAP:H4D	2.21	0.41
1:B:140:MET:CE	1:B:144:PHE:HB3	2.51	0.40
1:C:189:ALA:HB2	1:D:189:ALA:HB2	2.03	0.40
1:A:42:ALA:HB3	1:A:63:VAL:HB	2.03	0.40
1:C:233:MET:HG2	4:C:467:HOH:O	2.21	0.40
1:A:212:LEU:HB3	1:A:255:GLU:HG2	2.03	0.40
1:B:207:ASN:ND2	4:B:295:HOH:O	2.54	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	267/286 (93%)	248 (93%)	16 (6%)	3 (1%)	17	13
1	B	263/286 (92%)	246 (94%)	16 (6%)	1 (0%)	39	43
1	C	253/286 (88%)	238 (94%)	13 (5%)	2 (1%)	24	21
1	D	251/286 (88%)	232 (92%)	16 (6%)	3 (1%)	16	11
All	All	1034/1144 (90%)	964 (93%)	61 (6%)	9 (1%)	21	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	ILE
1	D	263	TRP
1	A	228	SER
1	D	280	TYR
1	C	202	SER
1	C	279	LEU
1	D	65	ALA
1	A	231	VAL
1	B	65	ALA

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	226/243 (93%)	214 (95%)	12 (5%)	28	30
1	B	222/243 (91%)	212 (96%)	10 (4%)	34	38
1	C	215/243 (88%)	200 (93%)	15 (7%)	19	17
1	D	211/243 (87%)	197 (93%)	14 (7%)	21	20
All	All	874/972 (90%)	823 (94%)	51 (6%)	24	25

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	61	VAL

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Mol	Chain	Res	Type
1	A	130	HIS
1	A	179	MET
1	A	221	GLU
1	A	224	MET
1	A	232	HIS
1	A	233	MET
1	A	265	THR
1	A	270	ASN
1	A	279	LEU
1	A	287	ASP
1	B	80	GLU
1	B	109	LEU
1	B	119	ASN
1	B	145	LEU
1	B	171	LEU
1	B	207	ASN
1	B	231	VAL
1	B	234	GLN
1	B	267	LEU
1	B	269	ARG
1	C	24	ASN
1	C	28	ARG
1	C	44	LYS
1	C	69	GLU
1	C	131	ASP
1	C	199	LYS
1	C	205	ARG
1	C	222	THR
1	C	225	LYS
1	C	233	MET
1	C	262	LEU
1	C	265	THR
1	C	270	ASN
1	C	278	PHE
1	C	279	LEU
1	D	123	ASN
1	D	125	SER
1	D	138	LYS
1	D	145	LEU
1	D	170	SER
1	D	220	THR
1	D	228	SER

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Mol	Chain	Res	Type
1	D	232	HIS
1	D	262	LEU
1	D	263	TRP
1	D	265	THR
1	D	269	ARG
1	D	270	ASN
1	D	279	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	123	ASN
1	A	270	ASN
1	B	119	ASN
1	B	120	HIS
1	B	160	GLN
1	B	207	ASN
1	C	24	ASN
1	C	101	GLN
1	C	120	HIS
1	C	123	ASN
1	C	234	GLN
1	C	270	ASN
1	D	53	HIS
1	D	120	HIS
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 (i)

8 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	NAP	A	1	-	42,52,52	1.53	2 (4%)	54,80,80	2.03	7 (12%)
3	A21	A	293	-	22,22,22	1.65	4 (18%)	22,34,34	1.76	5 (22%)
2	NAP	B	2	-	42,52,52	1.59	5 (11%)	54,80,80	2.55	8 (14%)
3	A21	B	293	-	22,22,22	1.96	5 (22%)	22,34,34	1.42	4 (18%)
3	A21	C	293	-	22,22,22	1.69	3 (13%)	22,34,34	1.67	6 (27%)
2	NAP	C	3	-	42,52,52	1.51	3 (7%)	54,80,80	2.04	7 (12%)
3	A21	D	293	-	22,22,22	2.19	6 (27%)	22,34,34	1.52	6 (27%)
2	NAP	D	4	-	42,52,52	1.57	3 (7%)	54,80,80	1.96	4 (7%)

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	NAP	A	1	-	-	0/27/67/67	0/5/5/5
3	A21	A	293	-	-	0/17/32/32	0/2/2/2
2	NAP	B	2	-	-	0/27/67/67	0/5/5/5
3	A21	B	293	-	-	0/17/32/32	0/2/2/2
3	A21	C	293	-	-	0/17/32/32	0/2/2/2
2	NAP	C	3	-	-	0/27/67/67	0/5/5/5
3	A21	D	293	-	-	0/17/32/32	0/2/2/2
2	NAP	D	4	-	-	0/27/67/67	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	293	A21	C11-S1	-7.79	1.67	1.75
3	B	293	A21	C11-S1	-7.04	1.68	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	293	A21	C11-S1	-5.25	1.70	1.75
3	C	293	A21	C11-S1	-4.98	1.70	1.75
3	C	293	A21	C8-S1	-3.79	1.76	1.84
3	D	293	A21	C8-S1	-3.78	1.76	1.84
3	B	293	A21	C8-S1	-3.34	1.77	1.84
3	A	293	A21	C8-S1	-3.33	1.77	1.84
3	C	293	A21	C11-N2	-2.96	1.27	1.31
3	D	293	A21	C11-N2	-2.92	1.27	1.31
3	D	293	A21	C13-N2	-2.72	1.32	1.38
3	B	293	A21	C6-C1	-2.65	1.48	1.52
3	B	293	A21	C13-N2	-2.41	1.33	1.38
3	A	293	A21	C13-N2	-2.30	1.33	1.38
3	D	293	A21	C8-C13	-2.23	1.51	1.53
3	A	293	A21	C11-N2	-2.12	1.28	1.31
3	B	293	A21	C11-N2	-2.10	1.28	1.31
3	D	293	A21	C6-C1	-2.08	1.49	1.52
2	C	3	NAP	C2A-N1A	2.00	1.37	1.33
2	D	4	NAP	C2A-N1A	2.04	1.37	1.33
2	B	2	NAP	C2A-N1A	2.20	1.38	1.33
2	B	2	NAP	PN-O5D	2.30	1.69	1.59
2	B	2	NAP	C3N-C7N	2.52	1.54	1.50
2	C	3	NAP	C2A-N3A	2.72	1.37	1.32
2	A	1	NAP	C2A-N3A	2.84	1.37	1.32
2	D	4	NAP	C2A-N3A	3.23	1.37	1.32
2	B	2	NAP	C2A-N3A	3.24	1.37	1.32
2	B	2	NAP	O7N-C7N	6.85	1.38	1.24
2	C	3	NAP	O7N-C7N	7.54	1.40	1.24
2	D	4	NAP	O7N-C7N	7.93	1.41	1.24
2	A	1	NAP	O7N-C7N	7.98	1.41	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAP	N3A-C2A-N1A	-15.96	116.67	128.89
2	D	4	NAP	N3A-C2A-N1A	-11.97	119.73	128.89
2	C	3	NAP	N3A-C2A-N1A	-11.26	120.28	128.89
2	A	1	NAP	N3A-C2A-N1A	-10.79	120.64	128.89
3	A	293	A21	N3-C11-N2	-5.38	119.17	124.25
3	C	293	A21	F3-C2-C8	-3.76	107.24	112.06
3	C	293	A21	N3-C11-N2	-3.56	120.89	124.25
2	B	2	NAP	C1B-N9A-C4A	-3.50	121.66	126.94
3	B	293	A21	C3-C1-C6	-3.39	108.05	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	293	A21	F1-C2-C8	-3.35	107.76	112.06
2	A	1	NAP	C1B-N9A-C4A	-3.31	121.94	126.94
3	A	293	A21	F3-C2-C8	-3.20	107.96	112.06
2	C	3	NAP	O2B-P2B-O1X	-3.12	99.32	107.11
3	D	293	A21	N3-C11-N2	-2.92	121.50	124.25
2	C	3	NAP	O7N-C7N-C3N	-2.89	116.43	119.59
3	B	293	A21	C19-C18-C6	-2.89	120.54	123.67
3	D	293	A21	C3-C1-C6	-2.79	108.65	111.40
3	B	293	A21	N3-C11-N2	-2.68	121.72	124.25
3	D	293	A21	F4-C2-C8	-2.60	108.72	112.06
3	C	293	A21	C19-C18-C6	-2.49	120.97	123.67
2	D	4	NAP	O3B-C3B-C2B	-2.49	103.98	111.16
3	D	293	A21	F3-C2-C8	-2.44	108.92	112.06
2	B	2	NAP	C4A-C5A-N7A	-2.38	107.28	109.48
2	C	3	NAP	O3B-C3B-C2B	-2.37	104.32	111.16
2	A	1	NAP	C4A-C5A-N7A	-2.33	107.34	109.48
3	D	293	A21	C19-C18-C6	-2.24	121.24	123.67
3	A	293	A21	C19-C18-C6	-2.22	121.27	123.67
2	A	1	NAP	O3-PA-O5B	-2.16	97.20	102.94
2	C	3	NAP	C4A-C5A-N7A	-2.15	107.50	109.48
3	C	293	A21	C3-C1-C6	-2.11	109.31	111.40
2	B	2	NAP	O2N-PN-O1N	2.02	123.48	112.53
2	B	2	NAP	P2B-O2B-C2B	2.06	126.50	121.56
3	D	293	A21	C22-C6-C18	2.17	119.10	116.14
2	D	4	NAP	O4B-C1B-N9A	2.30	112.90	108.10
3	A	293	A21	C22-C6-C18	2.35	119.34	116.14
3	C	293	A21	C22-C6-C18	2.41	119.42	116.14
2	A	1	NAP	O2N-PN-O1N	2.45	125.81	112.53
3	B	293	A21	C22-C6-C18	2.45	119.48	116.14
2	B	2	NAP	O4B-C1B-N9A	2.85	114.07	108.10
2	B	2	NAP	O4D-C1D-N1N	3.28	111.74	108.13
3	C	293	A21	C3-C1-N3	3.31	113.76	109.03
2	A	1	NAP	O4D-C1D-N1N	4.01	112.54	108.13
2	D	4	NAP	O4D-C1D-N1N	4.14	112.68	108.13
2	B	2	NAP	C3N-C7N-N7N	4.22	122.44	117.82
2	A	1	NAP	O4B-C1B-N9A	4.39	117.30	108.10
2	C	3	NAP	C3N-C7N-N7N	4.53	122.78	117.82
2	C	3	NAP	O4D-C1D-N1N	4.56	113.14	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAP	1	0
2	C	3	NAP	1	0
2	D	4	NAP	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, 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	263/286 (91%)	0.27	21 (7%)	15	16	29, 48, 76, 87	0
1	B	262/286 (91%)	0.29	19 (7%)	18	19	28, 48, 69, 84	0
1	C	254/286 (88%)	0.30	20 (7%)	15	17	31, 46, 73, 84	0
1	D	254/286 (88%)	0.89	44 (17%)	2	2	32, 62, 85, 89	0
All	All	1033/1144 (90%)	0.44	104 (10%)	9	10	28, 50, 79, 89	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	LEU	6.9
1	D	263	TRP	6.5
1	C	263	TRP	6.1
1	C	262	LEU	5.3
1	D	280	TYR	5.1
1	C	278	PHE	5.0
1	D	262	LEU	5.0
1	D	278	PHE	4.9
1	D	168	VAL	4.8
1	D	232	HIS	4.6
1	A	263	TRP	4.2
1	B	282	THR	4.0
1	B	24	ASN	3.9
1	D	71	LEU	3.9
1	A	278	PHE	3.8
1	B	190	LEU	3.7
1	C	205	ARG	3.7
1	D	281	SER	3.7
1	C	233	MET	3.6
1	D	166	VAL	3.6
1	D	231	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	205	ARG	3.5
1	D	28	ARG	3.5
1	B	22	PRO	3.5
1	C	282	THR	3.5
1	A	229	GLY	3.4
1	A	30	GLU	3.4
1	D	167	VAL	3.4
1	B	134	HIS	3.4
1	B	262	LEU	3.3
1	D	27	PHE	3.3
1	A	286	MET	3.2
1	D	203	VAL	3.2
1	B	26	GLU	3.1
1	C	281	SER	3.1
1	B	205	ARG	3.1
1	D	266	LEU	3.0
1	B	278	PHE	3.0
1	D	188	PHE	2.9
1	A	25	GLU	2.9
1	C	130	HIS	2.9
1	A	190	LEU	2.9
1	B	213	CYS	2.8
1	A	118	LEU	2.8
1	D	230	ILE	2.8
1	A	230	ILE	2.8
1	B	188	PHE	2.7
1	C	25	GLU	2.7
1	D	190	LEU	2.7
1	B	189	ALA	2.7
1	D	74	VAL	2.7
1	D	76	SER	2.6
1	C	207	ASN	2.6
1	D	240	GLU	2.6
1	B	212	LEU	2.6
1	D	187	LYS	2.6
1	D	147	TYR	2.6
1	D	26	GLU	2.6
1	C	185	ALA	2.6
1	A	207[A]	ASN	2.6
1	D	112	GLY	2.6
1	C	177[A]	TYR	2.6
1	B	214	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	206	VAL	2.5
1	D	30	GLU	2.5
1	C	203	VAL	2.5
1	D	72	GLN	2.5
1	B	169	SER	2.5
1	C	134	HIS	2.4
1	D	117	ILE	2.4
1	C	24	ASN	2.4
1	A	28	ARG	2.4
1	C	189	ALA	2.4
1	D	32	LEU	2.3
1	D	251	LEU	2.3
1	A	177[A]	TYR	2.3
1	D	118	LEU	2.3
1	B	184	SER	2.3
1	D	219	ASP	2.3
1	D	213	CYS	2.3
1	A	189	ALA	2.3
1	A	168	VAL	2.2
1	C	206	VAL	2.2
1	A	232	HIS	2.2
1	C	188	PHE	2.2
1	D	144	PHE	2.2
1	A	282	THR	2.2
1	C	190	LEU	2.2
1	A	192	GLY	2.2
1	B	173	GLY	2.2
1	C	173	GLY	2.1
1	D	189	ALA	2.1
1	D	39	VAL	2.1
1	D	212	LEU	2.1
1	D	121	ILE	2.1
1	D	156	PRO	2.1
1	D	214	VAL	2.1
1	A	233	MET	2.1
1	D	173	GLY	2.1
1	A	167	VAL	2.1
1	D	205	ARG	2.0
1	B	172	ALA	2.0
1	D	81	LEU	2.0
1	D	172	ALA	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
2	NAP	C	3	48/48	0.97	0.16	0.18	31,38,41,44	0
3	A21	B	293	21/21	0.97	0.15	-0.15	42,46,50,52	0
3	A21	D	293	21/21	0.95	0.16	-0.46	51,54,58,61	0
2	NAP	B	2	48/48	0.96	0.12	-0.68	30,33,43,46	0
2	NAP	A	1	48/48	0.97	0.10	-0.72	31,36,41,45	0
2	NAP	D	4	48/48	0.96	0.12	-0.94	47,52,57,60	0
3	A21	A	293	21/21	0.95	0.09	-1.01	39,43,45,47	0
3	A21	C	293	21/21	0.97	0.10	-1.14	39,45,49,52	0

6.5 Other polymers (i)

There are no such residues in this entry.