Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:02 AM GMT

PDB ID	:	3KM0
Title	:	17betaHSD1 in complex with 3beta-diol
Authors	:	Mazumdar, M.; Lin, S.-X.
Deposited on	:	2009-11-09
Resolution	:	2.30 Å(reported)

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

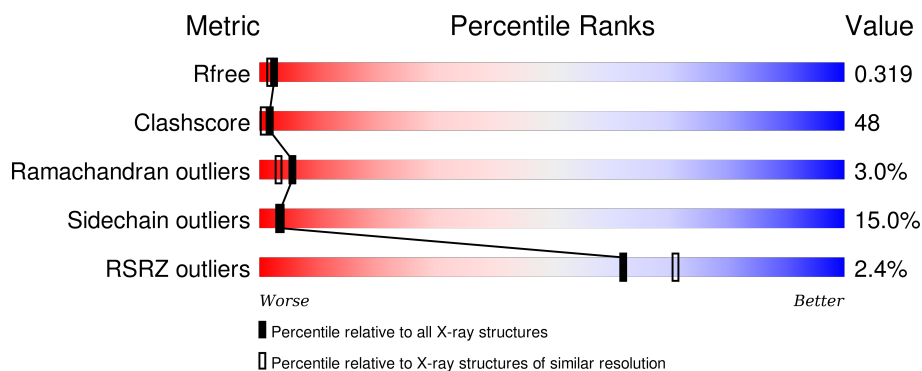|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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:
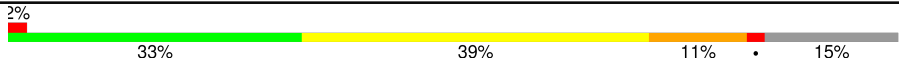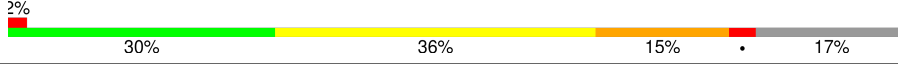*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Rfree		0.319
Clashscore		48
Ramachandran outliers		3.0%
Sidechain outliers		15.0%
RSRZ outliers		2.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	327	2% 33% 39% 11% • 15%
1	B	327	2% 30% 36% 15% • 17%

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:

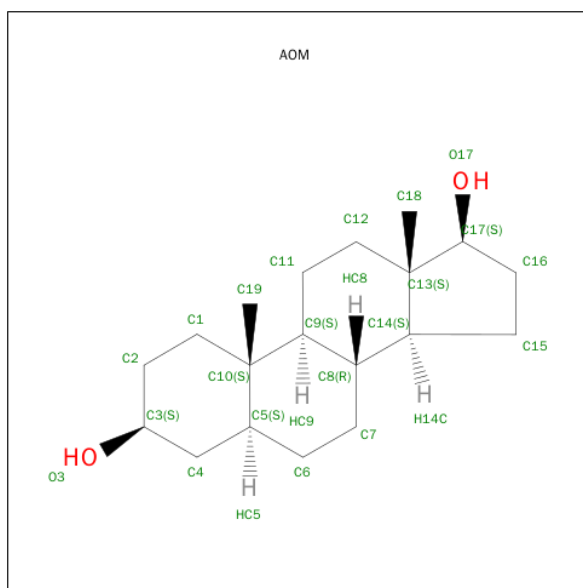| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AOM	C	1	-	-	-	X
2	AOM	D	1	-	-	X	X
3	NAP	E	360	-	-	X	X
3	NAP	F	360	-	-	X	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4544 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 Estradiol 17-beta-dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	4	0
			2125	1346	378	390	11			
1	B	272	Total	C	N	O	S	0	1	0
			2087	1324	372	380	11			

- Molecule 2 is 5-ALPHA-ANDROSTANE-3-BETA,17BETA-DIOL (three-letter code: AOM) (formula: $C_{19}H_{32}O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			21	19	2		
2	D	1	Total	C	O	0	0
			21	19	2		

- Molecule 3 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
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	B	95	Total	O	0	0
			95	95		
4	E	6	Total	O	0	0
			6	6		
4	F	2	Total	O	0	0
			2	2		

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: Estradiol 17-beta-dehydrogenase 1

Chain A:

• Molecule 1: Estradiol 17-beta-dehydrogenase 1

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.42Å 43.12Å 121.10Å 90.00° 128.59° 90.00°	Depositor
Resolution (Å)	18.98 – 2.30 18.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (18.98-2.30) 91.9 (18.98-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.233 , 0.312 0.241 , 0.319	Depositor DCC
R_{free} test set	1286 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 25.5	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	0 of 25732 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4544	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, AOM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	1.71	31/2164 (1.4%)	1.53	24/2936 (0.8%)
1	B	1.76	22/2125 (1.0%)	1.62	38/2882 (1.3%)
All	All	1.73	53/4289 (1.2%)	1.58	62/5818 (1.1%)

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	B	0	1
All	All	0	2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	GLU	CB-CG	-11.94	1.29	1.52
1	A	10	CYS	CB-SG	-10.10	1.65	1.82
1	B	119	VAL	CB-CG1	-8.89	1.34	1.52
1	A	214	ARG	CZ-NH1	7.24	1.42	1.33
1	A	119	VAL	CB-CG1	-7.17	1.37	1.52
1	B	9	GLY	C-O	6.98	1.34	1.23
1	A	170	ALA	CA-CB	-6.97	1.37	1.52
1	B	214	ARG	CB-CG	-6.78	1.34	1.52
1	A	253	TYR	CB-CG	-6.67	1.41	1.51
1	A	257	GLU	CG-CD	6.57	1.61	1.51
1	A	15	GLY	C-O	6.51	1.34	1.23
1	A	226	PHE	CE2-CZ	6.40	1.49	1.37
1	A	46	TRP	CB-CG	6.36	1.61	1.50
1	B	94	GLY	C-O	6.35	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	PHE	CE1-CZ	6.31	1.49	1.37
1	A	135	GLY	N-CA	-6.11	1.36	1.46
1	A	226	PHE	CD1-CE1	6.05	1.51	1.39
1	A	77	GLU	CB-CG	5.96	1.63	1.52
1	A	104	GLU	CG-CD	5.94	1.60	1.51
1	A	9	GLY	C-O	5.76	1.32	1.23
1	A	30	PHE	CE1-CZ	5.76	1.48	1.37
1	B	163	GLU	N-CA	5.75	1.57	1.46
1	B	51	ALA	CA-CB	5.71	1.64	1.52
1	B	252	ARG	C-O	5.68	1.34	1.23
1	B	226	PHE	CE1-CZ	5.67	1.48	1.37
1	B	9	GLY	N-CA	5.62	1.54	1.46
1	B	42	GLN	CB-CG	-5.61	1.37	1.52
1	B	216	TYR	CD1-CE1	5.59	1.47	1.39
1	A	266	ARG	CB-CG	-5.58	1.37	1.52
1	A	77	GLU	CG-CD	5.50	1.60	1.51
1	A	20	VAL	CB-CG1	5.45	1.64	1.52
1	A	46	TRP	CZ3-CH2	5.45	1.48	1.40
1	A	143	VAL	CB-CG2	5.39	1.64	1.52
1	B	240	PHE	CE1-CZ	5.39	1.47	1.37
1	B	81	GLU	CD-OE2	5.36	1.31	1.25
1	A	257	GLU	CB-CG	5.35	1.62	1.52
1	A	275	TYR	CD1-CE1	-5.29	1.31	1.39
1	B	160	PHE	CD2-CE2	5.28	1.49	1.39
1	B	38	ASP	CB-CG	-5.21	1.40	1.51
1	A	35	THR	N-CA	-5.19	1.35	1.46
1	A	73	ALA	CA-CB	5.16	1.63	1.52
1	A	33	TYR	CD1-CE1	5.15	1.47	1.39
1	A	240	PHE	CD2-CE2	5.13	1.49	1.39
1	B	61	THR	N-CA	-5.13	1.36	1.46
1	B	226	PHE	CD2-CE2	5.11	1.49	1.39
1	B	176	PHE	CG-CD2	5.10	1.46	1.38
1	B	214	ARG	CA-CB	-5.10	1.42	1.53
1	A	91	ALA	N-CA	5.09	1.56	1.46
1	B	160	PHE	CG-CD1	5.07	1.46	1.38
1	B	224	GLN	CG-CD	5.06	1.62	1.51
1	B	123	GLN	CG-CD	5.05	1.62	1.51
1	A	37[A]	ARG	CZ-NH1	5.03	1.39	1.33
1	A	93	LEU	N-CA	5.02	1.56	1.46

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	LEU	CB-CG-CD1	-10.81	92.62	111.00
1	B	252	ARG	NE-CZ-NH1	10.74	125.67	120.30
1	A	37[A]	ARG	NE-CZ-NH2	-10.69	114.96	120.30
1	B	146	LEU	CB-CG-CD1	-10.35	93.41	111.00
1	B	102	LEU	CB-CG-CD1	-10.19	93.68	111.00
1	B	62	LEU	CB-CG-CD2	-10.12	93.80	111.00
1	A	266	ARG	NE-CZ-NH1	-10.02	115.29	120.30
1	A	258	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	A	214	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	B	214	ARG	NE-CZ-NH1	-8.18	116.21	120.30
1	B	44	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	262	LEU	CA-CB-CG	7.76	133.14	115.30
1	A	100	GLU	CB-CA-C	-7.69	95.01	110.40
1	B	38	ASP	CB-CG-OD1	-7.69	111.38	118.30
1	B	206	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	37[A]	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	76	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	43	GLY	C-N-CA	-7.37	103.28	121.70
1	B	21	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	B	162	LEU	CB-CG-CD1	-7.30	98.60	111.00
1	B	121	MET	CG-SD-CE	7.29	111.86	100.20
1	A	162	LEU	CB-CG-CD1	-7.04	99.02	111.00
1	A	22	LEU	CA-CB-CG	7.01	131.43	115.30
1	A	266	ARG	NE-CZ-NH2	6.97	123.79	120.30
1	A	113	VAL	CG1-CB-CG2	-6.89	99.87	110.90
1	A	37[A]	ARG	N-CA-CB	6.80	122.84	110.60
1	B	21	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	B	87	LEU	CA-CB-CG	6.53	130.32	115.30
1	A	149	LEU	CB-CG-CD2	6.38	121.85	111.00
1	A	47	GLU	CA-CB-CG	6.33	127.32	113.40
1	B	186	GLY	N-CA-C	-6.30	97.36	113.10
1	B	70	LYS	CD-CE-NZ	-6.20	97.44	111.70
1	B	189	HIS	N-CA-CB	6.10	121.58	110.60
1	B	216	TYR	N-CA-C	-6.07	94.61	111.00
1	B	120	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	B	174	LEU	CB-CG-CD2	5.86	120.96	111.00
1	A	76	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	102	LEU	CB-CG-CD2	5.78	120.82	111.00
1	B	214	ARG	NH1-CZ-NH2	5.75	125.73	119.40
1	B	83	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	122	LEU	CB-CG-CD2	5.69	120.67	111.00
1	B	44	ARG	CA-CB-CG	5.62	125.75	113.40
1	B	206	ARG	NE-CZ-NH2	-5.60	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	44	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	162	LEU	CB-CA-C	-5.52	99.72	110.20
1	B	38	ASP	CB-CA-C	-5.50	99.40	110.40
1	B	235	GLU	CA-CB-CG	5.48	125.46	113.40
1	A	214	ARG	NH1-CZ-NH2	5.44	125.38	119.40
1	B	214	ARG	CB-CG-CD	-5.39	97.58	111.60
1	B	266	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	235	GLU	CA-CB-CG	-5.36	101.61	113.40
1	A	189	HIS	CB-CA-C	-5.35	99.70	110.40
1	B	173	LEU	CB-CG-CD1	-5.35	101.91	111.00
1	B	162	LEU	CA-CB-CG	5.33	127.57	115.30
1	B	96	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	110	VAL	CG1-CB-CG2	-5.32	102.38	110.90
1	B	76	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	241	LEU	CB-CG-CD2	5.24	119.91	111.00
1	A	208	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	A	190[A]	THR	N-CA-C	-5.16	97.08	111.00
1	B	64	LEU	CA-CB-CG	5.07	126.97	115.30
1	B	175	PRO	C-N-CA	-5.07	109.03	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	VAL	Peptide
1	B	270	PRO	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	2125	0	2157	183	11
1	B	2087	0	2125	231	1
2	C	21	0	32	6	0
2	D	21	0	32	15	0
3	E	48	0	25	42	0
3	F	48	0	25	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	91	0	0	22	1
4	B	95	0	0	36	1
4	E	6	0	0	6	0
4	F	2	0	0	3	0
All	All	4544	0	4396	424	12

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 48.

All (424) 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:279:MET:CE	1:A:283:VAL:HG23	1.38	1.51
1:A:279:MET:CE	1:A:283:VAL:CG2	2.02	1.37
1:A:270:PRO:HD3	4:A:402:HOH:O	1.20	1.29
1:B:14:ILE:HD12	3:E:360:NAP:O2N	1.30	1.28
1:A:37[A]:ARG:NH2	1:A:67:ARG:HH22	1.35	1.24
1:B:276:VAL:HG12	4:B:383:HOH:O	1.36	1.22
3:E:360:NAP:H51A	4:E:44:HOH:O	1.37	1.21
1:B:10:CYS:SG	4:B:395:HOH:O	1.94	1.21
3:E:360:NAP:H2D	4:E:86:HOH:O	1.43	1.18
1:A:37[A]:ARG:HG2	1:A:38:ASP:OD2	1.40	1.18
1:A:279:MET:HE1	1:A:283:VAL:CG2	1.76	1.15
1:B:92:GLY:HA3	4:E:113:HOH:O	0.99	1.14
1:B:260:LEU:N	1:B:260:LEU:HD12	1.62	1.13
1:A:185:CYS:HB2	3:F:360:NAP:C5N	1.80	1.12
1:A:279:MET:HE3	1:A:283:VAL:HG23	1.17	1.11
1:A:199:SER:O	1:A:202:GLU:OE1	1.71	1.09
1:B:74:ALA:O	1:B:77:GLU:HG2	1.52	1.08
1:A:227:ARG:HG3	1:A:227:ARG:HH11	0.90	1.03
1:B:232:ASN:OD1	1:B:235:GLU:HG2	1.57	1.03
2:D:1:AOM:HC3	3:E:360:NAP:C4N	1.90	1.02
1:A:66:VAL:HG22	3:F:360:NAP:N1A	1.74	1.01
1:B:260:LEU:CD1	1:B:260:LEU:H	1.74	1.00
1:B:214:ARG:HA	4:B:390:HOH:O	1.59	1.00
1:A:248:LYS:HG2	4:A:351:HOH:O	1.61	1.00
1:A:9:GLY:HA2	3:F:360:NAP:O2X	1.61	1.00
1:A:227:ARG:HG3	1:A:227:ARG:NH1	1.64	0.99
3:E:360:NAP:H3D	4:E:113:HOH:O	1.62	0.99
1:B:90:ASN:HA	1:B:140:THR:CG2	1.92	0.99
1:A:37[A]:ARG:NH2	1:A:67:ARG:NH2	2.09	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:HD3	4:A:403:HOH:O	1.64	0.98
1:B:9:GLY:HA2	3:E:360:NAP:O2X	1.63	0.98
1:A:279:MET:HE2	1:A:283:VAL:HG23	1.44	0.97
1:A:227:ARG:CG	1:A:227:ARG:HH11	1.80	0.95
1:A:263:LEU:O	1:A:263:LEU:HD22	1.67	0.95
1:B:260:LEU:N	1:B:260:LEU:CD1	2.27	0.94
1:B:180:LEU:C	1:B:180:LEU:HD23	1.87	0.94
1:B:185:CYS:HB2	3:E:360:NAP:C5N	1.98	0.93
1:A:132:ARG:CD	4:A:403:HOH:O	2.16	0.93
1:A:136:ARG:NH1	1:A:249:PRO:HG3	1.85	0.92
1:B:90:ASN:HA	1:B:140:THR:HG23	1.52	0.92
2:D:1:AOM:C3	3:E:360:NAP:C4N	2.47	0.91
1:B:244:LEU:C	1:B:244:LEU:HD12	1.91	0.91
1:B:264:ARG:HA	1:B:267:LEU:HD12	1.53	0.91
1:B:27:SER:O	1:B:28:GLN:HB2	1.70	0.90
1:A:267:LEU:HD22	1:B:267:LEU:HD23	1.54	0.90
1:A:279:MET:HE2	1:A:283:VAL:CG2	1.98	0.88
1:B:103:GLY:HA3	4:B:366:HOH:O	1.72	0.88
1:B:258:ARG:HH11	1:B:258:ARG:HB2	1.38	0.87
1:B:174:LEU:HB3	1:B:175:PRO:HD3	1.55	0.87
2:D:1:AOM:O3	3:E:360:NAP:C5N	2.21	0.87
1:B:185:CYS:HB2	3:E:360:NAP:C6N	2.04	0.86
1:B:263:LEU:HD13	1:B:267:LEU:HD11	1.55	0.86
2:D:1:AOM:HC3	3:E:360:NAP:H4N	1.57	0.86
1:A:279:MET:CE	1:A:283:VAL:HG21	2.06	0.85
1:B:224:GLN:O	1:B:228:GLU:HG3	1.77	0.85
1:A:78:ARG:CG	1:A:78:ARG:HH11	1.89	0.85
1:B:222:SER:HB3	2:D:1:AOM:H121	1.58	0.83
1:A:185:CYS:HB2	3:F:360:NAP:C6N	2.08	0.83
1:A:37[A]:ARG:CZ	1:A:67:ARG:NH2	2.42	0.82
1:B:105:ASP:O	1:B:109:SER:HB2	1.78	0.82
1:B:9:GLY:HA2	3:E:360:NAP:P2B	2.19	0.82
1:B:205:ASP:HA	4:B:333:HOH:O	1.80	0.82
2:D:1:AOM:O3	3:E:360:NAP:C4N	2.29	0.81
1:A:257:GLU:CG	1:A:260:LEU:HD22	2.12	0.80
1:A:185:CYS:HB2	3:F:360:NAP:H5N	1.62	0.80
1:B:281:ARG:NH2	1:B:282:GLU:HG2	1.96	0.80
1:B:91:ALA:HB1	3:E:360:NAP:C4A	2.12	0.80
1:B:11:SER:HB3	1:B:36:LEU:HD23	1.63	0.79
1:B:180:LEU:HD23	1:B:181:SER:N	1.98	0.77
1:B:76:ARG:HH11	1:B:76:ARG:HG2	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLU:O	1:B:260:LEU:HD13	1.85	0.77
1:B:50:ARG:HA	1:B:50:ARG:NE	1.98	0.77
1:B:213:HIS:C	4:B:390:HOH:O	2.23	0.76
1:A:174:LEU:N	1:A:175:PRO:CD	2.48	0.76
1:B:91:ALA:CB	3:E:360:NAP:N3A	2.49	0.76
1:B:213:HIS:ND1	4:B:390:HOH:O	2.19	0.76
1:B:258:ARG:NH1	1:B:258:ARG:HB2	2.00	0.76
1:B:34:ALA:CA	4:B:395:HOH:O	2.34	0.76
1:B:101:ALA:O	1:B:206:ARG:HD3	1.86	0.75
1:A:279:MET:HE1	1:A:283:VAL:HG21	1.64	0.75
1:A:147:MET:HE1	1:A:263:LEU:HB2	1.68	0.75
1:A:190[A]:THR:HA	4:A:378:HOH:O	1.87	0.74
1:B:34:ALA:HA	4:B:395:HOH:O	1.86	0.74
1:A:174:LEU:N	1:A:175:PRO:HD3	1.99	0.74
1:B:128:ASP:O	1:B:132:ARG:HG3	1.86	0.74
1:A:270:PRO:CD	4:A:402:HOH:O	1.97	0.74
1:B:90:ASN:OD1	1:B:140:THR:HG21	1.87	0.74
1:A:183:ILE:O	4:A:399:HOH:O	2.05	0.74
1:A:257:GLU:HG2	1:A:260:LEU:CD2	2.18	0.73
1:A:221:HIS:NE2	2:C:1:AOM:O17	2.22	0.73
1:A:190[A]:THR:CA	4:A:378:HOH:O	2.36	0.73
1:B:121:MET:HE3	1:B:125:PHE:CE1	2.23	0.73
1:B:66:VAL:HG22	3:E:360:NAP:N1A	2.03	0.72
1:A:185:CYS:SG	4:A:399:HOH:O	1.92	0.72
1:A:257:GLU:HA	1:A:260:LEU:HD22	1.70	0.72
1:A:257:GLU:HG3	1:A:260:LEU:HD22	1.70	0.72
1:A:78:ARG:NH1	4:A:339:HOH:O	2.23	0.72
1:B:14:ILE:CD1	3:E:360:NAP:O2N	2.26	0.71
1:A:186:GLY:O	3:F:360:NAP:H4N	1.90	0.71
1:B:91:ALA:HB1	3:E:360:NAP:N3A	2.05	0.71
1:B:213:HIS:CG	4:B:390:HOH:O	2.42	0.71
1:B:185:CYS:CB	3:E:360:NAP:C5N	2.68	0.71
1:A:136:ARG:NH2	1:A:246:ALA:O	2.21	0.71
1:A:93:LEU:HD21	1:A:113:VAL:HG11	1.71	0.71
1:A:267:LEU:CD2	1:B:267:LEU:HD23	2.21	0.71
1:A:257:GLU:CG	1:A:260:LEU:CD2	2.68	0.70
1:A:161:ALA:HB2	1:B:161:ALA:HB2	1.74	0.70
1:B:140:THR:HB	1:B:240:PHE:HZ	1.55	0.70
1:A:37[A]:ARG:HH21	1:A:67:ARG:HH22	1.39	0.70
1:A:202:GLU:O	1:A:205:ASP:HB2	1.91	0.70
1:B:222:SER:HB3	2:D:1:AOM:C12	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:HG22	3:F:360:NAP:C6A	2.22	0.70
1:B:111:LEU:HD23	1:B:158:SER:HB3	1.73	0.70
1:A:104:GLU:HG3	4:B:403:HOH:O	1.91	0.69
1:A:147:MET:CE	1:A:263:LEU:HB2	2.22	0.69
1:B:244:LEU:CD1	1:B:244:LEU:C	2.61	0.69
1:B:27:SER:O	1:B:28:GLN:CB	2.41	0.69
1:B:121:MET:CE	1:B:125:PHE:CE1	2.76	0.68
1:B:277:THR:N	4:B:383:HOH:O	2.26	0.68
1:A:123:GLN:NE2	4:A:329:HOH:O	2.27	0.68
1:A:267:LEU:HD22	1:B:267:LEU:CD2	2.23	0.67
1:A:9:GLY:HA2	3:F:360:NAP:P2B	2.34	0.67
1:B:21:ARG:HG3	1:B:21:ARG:HH11	1.60	0.67
1:B:260:LEU:HD13	1:B:260:LEU:H	1.58	0.67
1:B:214:ARG:N	4:B:390:HOH:O	2.26	0.67
1:B:210:HIS:NE2	4:B:396:HOH:O	2.28	0.67
1:B:66:VAL:HG13	3:E:360:NAP:H2A	1.78	0.66
1:B:44:ARG:HB3	1:B:44:ARG:NH1	2.09	0.66
1:B:239:VAL:HG21	1:B:255:THR:HG22	1.76	0.66
1:A:131:ARG:HH11	1:A:131:ARG:HG3	1.60	0.66
1:B:90:ASN:ND2	3:E:360:NAP:O2A	2.24	0.66
1:A:91:ALA:HB1	3:F:360:NAP:C4A	2.26	0.66
1:A:257:GLU:O	1:A:260:LEU:HB2	1.95	0.66
1:B:276:VAL:C	4:B:383:HOH:O	2.34	0.66
1:B:260:LEU:O	1:B:264:ARG:HD3	1.95	0.65
1:A:153:ASP:OD1	4:A:357:HOH:O	2.14	0.65
1:B:185:CYS:HB2	3:E:360:NAP:H5N	1.75	0.65
1:B:121:MET:HE3	1:B:125:PHE:HE1	1.61	0.65
1:A:281:ARG:NH1	4:A:352:HOH:O	2.30	0.65
1:B:187:PRO:HB3	1:B:226:PHE:CE1	2.32	0.65
1:A:167:GLU:O	1:A:171:VAL:HG23	1.96	0.65
1:A:167:GLU:OE1	1:B:266:ARG:NH2	2.29	0.65
1:B:50:ARG:CA	1:B:50:ARG:NE	2.59	0.65
1:A:5:VAL:HG13	1:A:86:VAL:HB	1.79	0.65
1:B:174:LEU:CB	1:B:175:PRO:HD3	2.25	0.65
1:B:2:ARG:HG2	1:B:29:SER:HA	1.79	0.64
1:A:201:GLU:O	1:A:203:VAL:N	2.30	0.64
1:B:50:ARG:HE	1:B:50:ARG:HA	1.61	0.64
1:A:77:GLU:CB	4:A:355:HOH:O	2.45	0.64
1:B:167:GLU:HG3	1:B:251:LEU:HD21	1.79	0.64
1:B:274:ASN:O	1:B:277:THR:N	2.31	0.64
1:B:83:ARG:HG3	1:B:83:ARG:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ARG:C	1:B:52:LEU:H	2.00	0.63
1:B:66:VAL:HG13	3:E:360:NAP:C2A	2.28	0.63
1:A:266:ARG:NH2	1:B:167:GLU:OE1	2.31	0.63
1:B:42:GLN:O	1:B:44:ARG:N	2.32	0.63
1:A:191[A]:ALA:O	4:A:415:HOH:O	2.15	0.63
1:B:2:ARG:HG2	1:B:29:SER:C	2.19	0.63
1:A:78:ARG:NH1	1:A:78:ARG:HG2	2.15	0.62
1:B:36:LEU:HA	3:E:360:NAP:O2X	2.00	0.62
1:A:191[A]:ALA:N	4:A:378:HOH:O	2.31	0.62
1:A:105:ASP:HB2	4:A:336:HOH:O	2.00	0.62
1:A:78:ARG:HG3	1:A:78:ARG:HH11	1.63	0.62
1:B:188:VAL:HB	3:E:360:NAP:C7N	2.29	0.62
1:B:121:MET:CE	1:B:125:PHE:HE1	2.11	0.62
1:A:270:PRO:CG	4:A:402:HOH:O	2.37	0.61
1:B:44:ARG:HB3	1:B:44:ARG:CZ	2.29	0.61
1:A:78:ARG:HG2	1:A:78:ARG:HH11	1.63	0.61
1:B:205:ASP:CA	4:B:333:HOH:O	2.41	0.61
1:A:257:GLU:HG2	1:A:260:LEU:HD23	1.82	0.61
1:A:121:MET:O	1:A:125:PHE:HD1	1.84	0.61
1:A:273:SER:HB3	1:B:250:THR:HG22	1.83	0.61
1:A:6:LEU:HD23	1:A:6:LEU:C	2.22	0.60
1:A:132:ARG:HD2	4:A:403:HOH:O	1.90	0.60
2:D:1:AOM:C3	3:E:360:NAP:C5N	2.78	0.60
1:B:95:LEU:HB2	1:B:110:VAL:HG21	1.82	0.60
1:A:100:GLU:OE1	1:A:207:THR:OG1	2.16	0.60
1:B:35:THR:N	4:B:395:HOH:O	2.34	0.60
1:B:188:VAL:HG23	3:E:360:NAP:C4N	2.31	0.60
1:B:258:ARG:CB	1:B:258:ARG:HH11	2.12	0.60
1:B:42:GLN:O	1:B:43:GLY:C	2.40	0.60
1:A:185:CYS:CB	3:F:360:NAP:C5N	2.70	0.59
1:A:91:ALA:CB	3:F:360:NAP:N3A	2.65	0.59
1:B:10:CYS:CB	4:B:395:HOH:O	2.37	0.59
1:B:281:ARG:CD	1:B:282:GLU:H	2.14	0.59
1:A:65:ASP:OD1	1:A:65:ASP:C	2.40	0.59
1:A:167:GLU:CD	1:B:266:ARG:HH21	2.05	0.59
1:B:70:LYS:HZ3	1:B:70:LYS:CB	2.16	0.59
1:A:201:GLU:O	1:A:202:GLU:C	2.38	0.59
1:B:16:LEU:C	1:B:16:LEU:HD23	2.23	0.59
1:B:142:SER:OG	2:D:1:AOM:HC41	2.02	0.59
1:B:66:VAL:HG22	3:E:360:NAP:C6A	2.32	0.59
1:A:245:ARG:NH1	4:A:397:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:CB	1:B:44:ARG:CZ	2.80	0.59
1:B:205:ASP:C	4:B:333:HOH:O	2.42	0.58
1:B:95:LEU:HD21	1:B:102:LEU:HD13	1.84	0.58
1:A:90:ASN:HA	1:A:140:THR:HG23	1.84	0.58
1:A:221:HIS:CD2	2:C:1:AOM:O17	2.56	0.58
1:B:39:LEU:O	1:B:41:THR:N	2.36	0.58
1:A:263:LEU:O	1:A:263:LEU:CD2	2.47	0.58
1:A:257:GLU:HG3	1:A:260:LEU:CD2	2.31	0.58
1:A:76:ARG:HH22	1:A:128:ASP:CB	2.16	0.58
1:B:138:LEU:CD2	1:B:181:SER:HB2	2.33	0.58
1:A:77:GLU:CA	4:A:355:HOH:O	2.51	0.58
1:B:274:ASN:O	1:B:275:TYR:C	2.43	0.58
1:B:281:ARG:HH21	1:B:282:GLU:HG2	1.66	0.58
1:A:33:TYR:OH	1:A:81:GLU:OE1	2.19	0.57
1:A:118:THR:HG21	1:A:162:LEU:HD21	1.86	0.57
1:B:210:HIS:N	1:B:210:HIS:CD2	2.72	0.57
1:B:91:ALA:HB2	3:E:360:NAP:N3A	2.19	0.57
1:B:214:ARG:CA	4:B:390:HOH:O	2.30	0.57
1:B:39:LEU:C	1:B:41:THR:N	2.57	0.57
1:A:21:ARG:O	1:A:21:ARG:NH1	2.36	0.57
1:B:76:ARG:HG2	1:B:76:ARG:NH1	2.16	0.57
1:A:25:ASP:OD2	1:A:27:SER:HB3	2.04	0.56
1:B:265:MET:SD	1:B:278:ALA:HB2	2.44	0.56
1:A:66:VAL:O	1:A:120:ARG:HD2	2.05	0.56
1:A:200:PRO:HA	1:A:203:VAL:HB	1.88	0.56
1:B:43:GLY:O	1:B:47:GLU:HB2	2.06	0.56
1:B:213:HIS:CE1	4:B:390:HOH:O	2.56	0.56
1:B:50:ARG:O	1:B:52:LEU:N	2.39	0.55
1:B:185:CYS:HB2	3:E:360:NAP:H6N	1.88	0.55
1:B:91:ALA:HA	3:E:360:NAP:O4B	2.07	0.55
1:B:39:LEU:C	1:B:41:THR:H	2.09	0.55
1:B:265:MET:SD	1:B:278:ALA:CB	2.95	0.55
1:B:141:GLY:O	3:E:360:NAP:H6N	2.06	0.55
1:B:180:LEU:C	1:B:180:LEU:CD2	2.63	0.55
1:B:14:ILE:HG12	1:B:236:VAL:HG11	1.89	0.55
1:B:256:THR:OG1	1:B:257:GLU:N	2.38	0.54
1:A:180:LEU:HD23	1:A:181:SER:N	2.23	0.54
2:D:1:AOM:O3	3:E:360:NAP:C6N	2.56	0.54
1:A:174:LEU:HG	1:A:174:LEU:O	2.08	0.54
1:A:270:PRO:O	1:B:252:ARG:HD2	2.08	0.54
1:B:10:CYS:HB2	4:B:395:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ASN:OD1	1:B:235:GLU:CG	2.44	0.53
1:A:78:ARG:CG	1:A:78:ARG:NH1	2.56	0.53
1:B:2:ARG:HG2	1:B:29:SER:O	2.07	0.53
1:A:91:ALA:HB2	3:F:360:NAP:N3A	2.23	0.53
1:A:186:GLY:O	3:F:360:NAP:C4N	2.55	0.53
1:B:245:ARG:NH2	4:B:399:HOH:O	2.41	0.53
1:B:17:HIS:CE1	1:B:234:GLU:OE2	2.62	0.53
1:B:166:CYS:HB2	1:B:182:LEU:HD11	1.91	0.53
1:A:206:ARG:HD3	4:A:379:HOH:O	2.09	0.53
1:B:257:GLU:OE2	1:B:260:LEU:HD22	2.09	0.52
1:B:50:ARG:C	1:B:52:LEU:N	2.61	0.52
1:A:180:LEU:HD23	1:A:181:SER:H	1.74	0.52
1:B:131:ARG:HG2	4:B:387:HOH:O	2.09	0.52
1:A:267:LEU:CD2	1:B:267:LEU:CD2	2.86	0.52
1:B:21:ARG:HG3	1:B:21:ARG:NH1	2.21	0.52
1:B:154:VAL:CG1	1:B:154:VAL:O	2.56	0.52
1:B:67:ARG:NH1	4:B:336:HOH:O	2.43	0.52
1:A:76:ARG:HH22	1:A:128:ASP:HB3	1.76	0.51
1:A:88:VAL:HA	1:A:138:LEU:O	2.10	0.51
1:A:279:MET:HE2	1:A:283:VAL:HG21	1.84	0.51
1:B:90:ASN:CA	1:B:140:THR:CG2	2.79	0.51
1:A:92:GLY:HA2	1:A:114:ASN:OD1	2.11	0.51
1:A:14:ILE:HG13	3:F:360:NAP:O2N	2.11	0.51
1:A:173:LEU:C	1:A:175:PRO:CD	2.79	0.51
1:A:259:PHE:CE1	2:C:1:AOM:H151	2.46	0.51
1:A:143:VAL:HB	2:C:1:AOM:HC61	1.93	0.51
1:B:136:ARG:NH1	1:B:249:PRO:HG2	2.25	0.51
3:E:360:NAP:C2D	4:E:86:HOH:O	2.24	0.51
1:B:281:ARG:NE	1:B:282:GLU:H	2.07	0.51
1:B:131:ARG:NH1	4:B:387:HOH:O	2.42	0.51
1:B:185:CYS:CB	3:E:360:NAP:C6N	2.85	0.50
1:B:214:ARG:HA	1:B:217:GLN:HB2	1.92	0.50
1:A:118:THR:HG21	1:A:162:LEU:CD2	2.41	0.50
1:B:264:ARG:CA	1:B:267:LEU:HD12	2.35	0.50
1:B:130:LYS:HZ3	1:B:173:LEU:CD2	2.24	0.50
1:A:254:PHE:CD1	1:A:254:PHE:N	2.80	0.50
3:F:360:NAP:H3D	4:F:52:HOH:O	2.11	0.50
1:A:201:GLU:C	1:A:203:VAL:N	2.64	0.50
1:A:258:ARG:HB2	1:A:258:ARG:HH11	1.77	0.50
1:A:141:GLY:O	3:F:360:NAP:H6N	2.12	0.49
1:A:225:VAL:HG21	2:C:1:AOM:H17C	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LYS:HZ3	1:B:70:LYS:HB3	1.76	0.49
1:B:216:TYR:O	1:B:217:GLN:C	2.48	0.49
1:A:221:HIS:CD2	2:C:1:AOM:HO17	2.25	0.49
1:B:143:VAL:O	1:B:146:LEU:HB2	2.13	0.49
1:B:232:ASN:HB2	1:B:233:PRO:HD2	1.94	0.49
1:A:68:ASP:O	1:A:72:VAL:HG23	2.13	0.49
1:B:244:LEU:HD12	1:B:244:LEU:O	2.12	0.49
1:A:5:VAL:HG12	1:A:6:LEU:N	2.27	0.48
1:A:239:VAL:HG12	1:A:239:VAL:O	2.14	0.48
1:A:167:GLU:OE2	1:B:266:ARG:NE	2.43	0.48
1:A:203:VAL:CG1	1:A:203:VAL:O	2.60	0.48
1:B:173:LEU:O	1:B:176:PHE:N	2.45	0.48
1:A:42:GLN:HE21	1:A:61:THR:HG21	1.79	0.48
1:A:94:GLY:HA2	1:A:155:TYR:CD1	2.49	0.48
1:B:8:THR:HA	1:B:35:THR:OG1	2.13	0.48
1:B:244:LEU:HD12	1:B:245:ARG:N	2.28	0.48
1:B:2:ARG:HG2	1:B:29:SER:CA	2.43	0.48
1:B:204:LEU:HB2	1:B:212:PHE:CE2	2.49	0.48
1:B:266:ARG:HA	1:B:275:TYR:HB2	1.96	0.48
1:A:136:ARG:HH12	1:A:249:PRO:HG3	1.75	0.48
1:B:83:ARG:HD2	4:B:378:HOH:O	2.14	0.48
1:B:92:GLY:O	1:B:93:LEU:HD23	2.14	0.47
3:E:360:NAP:O3X	4:E:79:HOH:O	2.20	0.47
1:B:210:HIS:H	1:B:210:HIS:CD2	2.33	0.47
1:A:95:LEU:HD23	1:A:154:VAL:HB	1.96	0.47
1:B:9:GLY:CA	3:E:360:NAP:O2X	2.49	0.47
1:A:257:GLU:CG	1:A:260:LEU:HD23	2.42	0.47
1:B:232:ASN:CB	1:B:233:PRO:HD2	2.45	0.47
1:A:11:SER:HB3	1:A:36:LEU:HD23	1.97	0.47
1:A:104:GLU:HA	4:B:403:HOH:O	2.14	0.47
1:B:2:ARG:NH2	4:B:359:HOH:O	2.27	0.47
1:A:209:ILE:HG23	1:A:210:HIS:ND1	2.30	0.47
1:A:6:LEU:HD22	1:A:87:LEU:CD1	2.45	0.47
1:A:175:PRO:HD2	1:A:176:PHE:HD1	1.80	0.46
1:B:167:GLU:HG3	1:B:251:LEU:CD2	2.44	0.46
1:B:263:LEU:O	1:B:267:LEU:HG	2.16	0.46
1:B:214:ARG:C	1:B:216:TYR:H	2.18	0.46
1:B:101:ALA:HA	1:B:206:ARG:HB3	1.97	0.46
1:A:135:GLY:O	1:A:178:VAL:HA	2.16	0.46
1:B:260:LEU:HD12	1:B:260:LEU:H	1.34	0.45
1:B:281:ARG:HD2	1:B:282:GLU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLN:NE2	4:B:369:HOH:O	2.20	0.45
1:B:244:LEU:CD1	1:B:244:LEU:O	2.64	0.45
1:A:77:GLU:OE2	1:A:78:ARG:NE	2.49	0.45
1:B:276:VAL:CG1	4:B:383:HOH:O	2.19	0.45
1:A:91:ALA:HB1	3:F:360:NAP:N3A	2.31	0.45
1:B:138:LEU:HD23	1:B:181:SER:HB2	1.99	0.45
1:A:104:GLU:CG	4:B:403:HOH:O	2.56	0.45
1:A:199:SER:N	1:A:202:GLU:OE1	2.50	0.45
1:A:173:LEU:C	1:A:175:PRO:HD2	2.36	0.45
1:A:126:LEU:O	1:A:127:PRO:C	2.55	0.45
1:B:259:PHE:C	1:B:260:LEU:HD12	2.32	0.45
1:A:260:LEU:N	1:A:261:PRO:HD2	2.32	0.45
1:B:50:ARG:NH2	1:B:53:ALA:HA	2.32	0.45
1:B:183:ILE:HG22	1:B:255:THR:CG2	2.46	0.45
1:B:259:PHE:CE1	2:D:1:AOM:H151	2.52	0.45
1:A:169:LEU:HA	4:B:355:HOH:O	2.17	0.45
1:B:42:GLN:C	1:B:44:ARG:N	2.71	0.45
1:A:279:MET:HE3	1:A:283:VAL:CG2	2.05	0.44
1:A:261:PRO:C	1:A:263:LEU:H	2.19	0.44
1:A:99:LEU:O	1:A:102:LEU:HB2	2.17	0.44
1:A:140:THR:HB	1:A:240:PHE:HZ	1.83	0.44
1:B:281:ARG:CZ	1:B:282:GLU:HG2	2.47	0.44
1:B:2:ARG:O	1:B:83:ARG:NH2	2.50	0.44
1:B:260:LEU:N	1:B:261:PRO:CD	2.81	0.44
1:B:44:ARG:HB2	1:B:44:ARG:CZ	2.47	0.44
1:A:34:ALA:O	1:A:61:THR:HA	2.17	0.44
1:B:90:ASN:HA	1:B:140:THR:HG21	1.92	0.44
2:D:1:AOM:HC3	3:E:360:NAP:C5N	2.43	0.44
1:B:50:ARG:HH22	1:B:53:ALA:HA	1.82	0.44
1:B:148:GLY:O	1:B:275:TYR:OH	2.36	0.43
1:B:173:LEU:O	1:B:174:LEU:C	2.56	0.43
1:B:38:ASP:HA	1:B:63:GLN:HE21	1.82	0.43
1:B:154:VAL:HG12	1:B:154:VAL:O	2.16	0.43
1:B:280:HIS:CE1	1:B:284:PHE:CD2	3.06	0.43
1:B:142:SER:OG	2:D:1:AOM:C4	2.67	0.43
1:A:175:PRO:CD	1:A:176:PHE:H	2.31	0.43
1:A:77:GLU:OE2	1:A:78:ARG:CD	2.67	0.43
1:A:6:LEU:HD22	1:A:87:LEU:HD12	2.00	0.43
1:B:16:LEU:HD22	1:B:17:HIS:CD2	2.54	0.43
1:A:131:ARG:NH1	1:A:131:ARG:HG3	2.32	0.43
1:B:34:ALA:HB1	4:B:395:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:VAL:HA	1:B:138:LEU:O	2.18	0.43
1:B:130:LYS:NZ	1:B:173:LEU:HD23	2.33	0.43
1:A:25:ASP:OD2	1:A:27:SER:CB	2.66	0.43
1:B:215:PHE:O	1:B:215:PHE:CG	2.69	0.43
1:B:207:THR:O	1:B:208:ASP:O	2.36	0.43
1:A:261:PRO:C	1:A:263:LEU:N	2.72	0.43
1:A:274:ASN:HA	1:A:274:ASN:HD22	1.59	0.43
1:B:257:GLU:C	1:B:260:LEU:HD13	2.37	0.43
1:B:214:ARG:NH2	4:B:345:HOH:O	2.51	0.43
1:A:271:SER:HB2	1:B:250:THR:HG21	2.01	0.43
1:A:37[A]:ARG:CZ	1:A:67:ARG:CZ	2.97	0.43
1:B:35:THR:HA	1:B:62:LEU:O	2.19	0.43
1:A:42:GLN:NE2	1:A:46:TRP:HE1	2.17	0.42
3:E:360:NAP:C5D	3:E:360:NAP:O5B	2.68	0.42
1:B:34:ALA:O	1:B:61:THR:HA	2.18	0.42
3:F:360:NAP:C2D	4:F:52:HOH:O	2.67	0.42
1:B:33:TYR:HA	1:B:60:GLU:O	2.19	0.42
1:A:47:GLU:OE2	1:A:47:GLU:HA	2.19	0.42
1:A:111:LEU:HD12	1:B:116:VAL:HG22	2.01	0.42
1:B:275:TYR:CD2	1:B:275:TYR:C	2.91	0.42
1:B:93:LEU:HD11	1:B:113:VAL:HG21	2.01	0.42
2:D:1:AOM:HC8	2:D:1:AOM:H182	1.79	0.42
1:B:276:VAL:CB	4:B:383:HOH:O	2.60	0.42
1:A:201:GLU:HB2	1:A:202:GLU:H	1.65	0.42
1:A:137:VAL:HB	1:A:180:LEU:HG	2.00	0.42
1:B:5:VAL:HA	1:B:86:VAL:O	2.19	0.42
1:A:175:PRO:HD2	1:A:176:PHE:CD1	2.55	0.42
1:B:283:VAL:O	1:B:283:VAL:HG12	2.20	0.42
1:B:263:LEU:O	1:B:267:LEU:HD12	2.20	0.42
1:B:210:HIS:O	1:B:214:ARG:HG3	2.19	0.42
1:B:16:LEU:C	1:B:16:LEU:CD2	2.87	0.42
1:A:87:LEU:HD11	1:A:121:MET:CE	2.50	0.42
1:A:121:MET:O	1:A:125:PHE:CD1	2.69	0.42
1:B:225:VAL:O	1:B:229:ALA:HB3	2.20	0.42
2:D:1:AOM:O3	3:E:360:NAP:C3N	2.69	0.41
1:A:188:VAL:HB	3:F:360:NAP:C7N	2.49	0.41
3:F:360:NAP:H2D	4:F:52:HOH:O	2.20	0.41
1:A:201:GLU:C	1:A:203:VAL:H	2.22	0.41
1:B:226:PHE:O	1:B:230:ALA:CB	2.68	0.41
1:B:39:LEU:CD1	1:B:63:GLN:HG3	2.50	0.41
1:A:23:ALA:HB3	1:A:54:CYS:SG	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PRO:HA	1:A:56:PRO:HD3	1.78	0.41
3:E:360:NAP:H52N	3:E:360:NAP:O5B	2.20	0.41
3:F:360:NAP:C5D	3:F:360:NAP:O5B	2.68	0.41
1:A:163:GLU:OE2	1:A:184:GLU:OE2	2.38	0.41
1:A:2:ARG:HB3	1:A:29:SER:O	2.20	0.41
1:B:65:ASP:HB3	1:B:68:ASP:HB3	2.02	0.41
3:F:360:NAP:O5B	3:F:360:NAP:H52N	2.20	0.41
1:B:121:MET:HE1	1:B:125:PHE:CE1	2.53	0.41
1:B:2:ARG:HB2	1:B:2:ARG:HE	1.57	0.41
1:B:96:LEU:HD11	1:B:218:TYR:CE2	2.55	0.41
1:A:35:THR:HG22	1:A:62:LEU:HB2	2.02	0.41
1:A:185:CYS:C	3:F:360:NAP:H5N	2.41	0.41
1:B:70:LYS:CB	1:B:70:LYS:NZ	2.74	0.41
1:B:247:PRO:HG2	1:B:248:LYS:H	1.86	0.41
1:B:46:TRP:CE3	1:B:46:TRP:HA	2.56	0.40
1:A:48:ALA:O	1:A:51:ALA:HB3	2.20	0.40
1:A:113:VAL:O	1:A:117:GLY:HA3	2.21	0.40
1:A:237:ALA:O	1:A:238:GLU:C	2.60	0.40
1:B:22:LEU:CD2	1:B:241:LEU:HD21	2.51	0.40
1:A:140:THR:OG1	3:F:360:NAP:O4D	2.40	0.40
1:B:25:ASP:HA	1:B:26:PRO:HD3	1.85	0.40
1:B:281:ARG:CD	1:B:282:GLU:N	2.82	0.40
1:B:70:LYS:HE2	1:B:70:LYS:HB3	1.93	0.40
1:A:96:LEU:HD12	1:A:97:GLY:N	2.36	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:CZ	1:A:255:THR:O[4_454]	0.56	1.64
1:A:50:ARG:NH2	1:A:256:THR:N[4_454]	0.61	1.59
1:A:50:ARG:NH1	1:A:255:THR:O[4_454]	0.78	1.42
1:A:50:ARG:NH2	1:A:255:THR:C[4_454]	0.88	1.32
1:A:50:ARG:CZ	1:A:255:THR:C[4_454]	1.12	1.08
1:A:50:ARG:NH1	1:A:255:THR:C[4_454]	1.54	0.66
1:A:50:ARG:NH2	1:A:256:THR:CA[4_454]	1.60	0.60
1:A:50:ARG:NE	1:A:255:THR:O[4_454]	1.66	0.54
1:A:50:ARG:NH2	1:A:255:THR:O[4_454]	1.66	0.54
1:A:50:ARG:CZ	1:A:256:THR:N[4_454]	1.90	0.30
1:A:214:ARG:NH2	4:A:370:HOH:O[2_554]	2.10	0.10
1:B:235:GLU:OE1	4:B:389:HOH:O[4_545]	2.15	0.05

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	274/327 (84%)	245 (89%)	24 (9%)	5 (2%)	11	9
1	B	268/327 (82%)	219 (82%)	38 (14%)	11 (4%)	3	1
All	All	542/654 (83%)	464 (86%)	62 (11%)	16 (3%)	5	3

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	THR
1	A	175	PRO
1	A	201	GLU
1	A	202	GLU
1	B	170	ALA
1	B	208	ASP
1	B	271	SER
1	B	282	GLU
1	B	40	LYS
1	B	43	GLY
1	B	205	ASP
1	B	274	ASN
1	B	203	VAL
1	B	163	GLU
1	B	268	ASP
1	A	127	PRO

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	229/257 (89%)	197 (86%)	32 (14%)	4	4
1	B	225/257 (88%)	189 (84%)	36 (16%)	3	3
All	All	454/514 (88%)	386 (85%)	68 (15%)	3	3

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	39	LEU
1	A	44	ARG
1	A	45	LEU
1	A	47	GLU
1	A	52	LEU
1	A	62	LEU
1	A	69	SER
1	A	77	GLU
1	A	78	ARG
1	A	93	LEU
1	A	127	PRO
1	A	131	ARG
1	A	140	THR
1	A	178	VAL
1	A	181	SER
1	A	199	SER
1	A	202	GLU
1	A	204	LEU
1	A	206	ARG
1	A	224	GLN
1	A	227	ARG
1	A	232	ASN
1	A	244	LEU
1	A	247	PRO
1	A	248	LYS
1	A	252	ARG
1	A	258	ARG
1	A	262	LEU
1	A	263	LEU
1	A	264	ARG
1	A	281	ARG
1	B	24	SER
1	B	28	GLN
1	B	38	ASP

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Mol	Chain	Res	Type
1	B	39	LEU
1	B	44	ARG
1	B	45	LEU
1	B	47	GLU
1	B	50	ARG
1	B	63	GLN
1	B	70	LYS
1	B	71	SER
1	B	76	ARG
1	B	100	GLU
1	B	105	ASP
1	B	109	SER
1	B	121	MET
1	B	130	LYS
1	B	140	THR
1	B	143	VAL
1	B	182	LEU
1	B	210	HIS
1	B	213	HIS
1	B	222	SER
1	B	224	GLN
1	B	235	GLU
1	B	239	VAL
1	B	244	LEU
1	B	248	LYS
1	B	249	PRO
1	B	252	ARG
1	B	260	LEU
1	B	262	LEU
1	B	263	LEU
1	B	264	ARG
1	B	271	SER
1	B	281	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	123	GLN
1	A	152	ASN
1	A	231	GLN
1	A	274	ASN

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Mol	Chain	Res	Type
1	B	17	HIS
1	B	123	GLN

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 ⓘ

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	$\#|Z| > 2$
2	AOM	C	1	-	24,24,24	1.00	1 (4%)	39,39,39	3.17	21 (53%)
2	AOM	D	1	-	24,24,24	0.90	0	39,39,39	2.72	24 (61%)
3	NAP	E	360	-	42,52,52	1.70	5 (11%)	54,80,80	2.59	14 (25%)
3	NAP	F	360	-	42,52,52	1.70	5 (11%)	54,80,80	2.59	14 (25%)

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	AOM	C	1	-	-	0/0/58/58	0/4/4/4
2	AOM	D	1	-	-	0/0/58/58	0/4/4/4
3	NAP	E	360	-	-	0/27/67/67	0/5/5/5
3	NAP	F	360	-	-	0/27/67/67	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	360	NAP	P2B-O2X	-6.35	1.31	1.54
3	F	360	NAP	P2B-O2X	-6.34	1.31	1.54
3	E	360	NAP	P2B-O2B	-5.03	1.44	1.60
3	F	360	NAP	P2B-O2B	-5.00	1.44	1.60
3	F	360	NAP	P2B-O1X	-3.91	1.38	1.51
3	E	360	NAP	P2B-O1X	-3.90	1.38	1.51
3	F	360	NAP	P2B-O3X	-3.18	1.43	1.54
3	E	360	NAP	P2B-O3X	-3.16	1.43	1.54
2	C	1	AOM	C8-C14	-2.70	1.48	1.53
3	F	360	NAP	PA-O2A	-2.08	1.46	1.54
3	E	360	NAP	PA-O2A	-2.05	1.46	1.54

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	360	NAP	N3A-C2A-N1A	-9.49	121.63	128.89
3	E	360	NAP	N3A-C2A-N1A	-9.47	121.64	128.89
2	C	1	AOM	C14-C13-C17	-6.67	92.15	99.28
2	C	1	AOM	C4-C5-C6	-5.72	100.98	111.66
2	C	1	AOM	C10-C9-C8	-5.55	106.21	112.40
2	C	1	AOM	O3-C3-C4	-5.22	99.48	109.86
2	D	1	AOM	C7-C6-C5	-4.83	102.13	111.92
2	C	1	AOM	C7-C8-C14	-4.76	104.14	112.02
2	D	1	AOM	C6-C7-C8	-4.45	104.14	112.10
2	D	1	AOM	C5-C4-C3	-4.44	106.31	112.91
2	C	1	AOM	C6-C7-C8	-4.02	104.91	112.10
3	F	360	NAP	O5B-C5B-C4B	-3.70	95.47	109.12
3	E	360	NAP	O5B-C5B-C4B	-3.69	95.50	109.12
2	D	1	AOM	C18-C13-C12	-3.69	104.25	110.54
2	D	1	AOM	C12-C13-C14	-3.58	101.48	107.31
2	D	1	AOM	C13-C14-C8	-3.54	108.83	114.37
3	E	360	NAP	C4B-O4B-C1B	-3.37	106.01	109.72
3	F	360	NAP	C4B-O4B-C1B	-3.32	106.07	109.72
2	C	1	AOM	C7-C6-C5	-3.28	105.26	111.92
3	E	360	NAP	C3N-C7N-N7N	-3.02	114.52	117.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	360	NAP	C3N-C7N-N7N	-2.94	114.60	117.82
2	D	1	AOM	C19-C10-C1	-2.93	103.28	108.20
2	C	1	AOM	C13-C14-C8	-2.92	109.81	114.37
3	E	360	NAP	C4A-C5A-N7A	-2.84	106.87	109.48
3	F	360	NAP	C4A-C5A-N7A	-2.80	106.90	109.48
2	D	1	AOM	O17-C17-C16	-2.78	105.26	111.56
2	C	1	AOM	C16-C15-C14	-2.70	99.69	105.12
2	C	1	AOM	C19-C10-C9	-2.50	107.44	111.18
2	D	1	AOM	C11-C9-C8	-2.47	108.16	111.74
2	D	1	AOM	O3-C3-C4	-2.25	105.40	109.86
2	C	1	AOM	C19-C10-C1	-2.22	104.47	108.20
2	D	1	AOM	C4-C3-C2	-2.15	107.78	110.52
2	C	1	AOM	C11-C9-C8	-2.06	108.75	111.74
3	E	360	NAP	C1B-N9A-C4A	-2.01	123.91	126.94
3	F	360	NAP	C1B-N9A-C4A	-2.01	123.92	126.94
2	D	1	AOM	C19-C10-C5	2.03	113.83	110.25
2	D	1	AOM	C18-C13-C14	2.04	115.75	111.75
2	D	1	AOM	C15-C16-C17	2.08	107.80	105.75
3	E	360	NAP	O4B-C4B-C5B	2.13	116.95	109.32
3	E	360	NAP	C2B-C3B-C4B	2.14	106.92	101.85
3	F	360	NAP	O4B-C4B-C5B	2.14	116.99	109.32
3	F	360	NAP	C2B-C3B-C4B	2.16	106.97	101.85
2	C	1	AOM	C4-C3-C2	2.18	113.30	110.52
2	D	1	AOM	C12-C11-C9	2.25	116.89	113.10
3	F	360	NAP	O3D-C3D-C2D	2.25	119.16	111.83
3	E	360	NAP	O3D-C3D-C2D	2.26	119.19	111.83
3	E	360	NAP	O5D-C5D-C4D	2.51	118.38	109.12
3	F	360	NAP	O5D-C5D-C4D	2.52	118.40	109.12
2	D	1	AOM	C6-C5-C10	2.56	116.99	112.26
3	E	360	NAP	O2B-C2B-C1B	2.62	120.23	110.02
3	F	360	NAP	O2B-C2B-C1B	2.63	120.26	110.02
2	D	1	AOM	C14-C13-C17	2.63	102.09	99.28
2	C	1	AOM	C15-C14-C13	2.70	107.33	103.82
2	D	1	AOM	C11-C9-C10	2.79	117.41	113.88
2	D	1	AOM	C4-C5-C10	2.82	115.76	112.66
2	C	1	AOM	C11-C12-C13	2.96	118.11	112.84
3	F	360	NAP	P2B-O2B-C2B	3.29	129.45	121.56
3	E	360	NAP	P2B-O2B-C2B	3.30	129.48	121.56
2	C	1	AOM	C1-C10-C9	3.59	117.24	111.45
2	C	1	AOM	C1-C2-C3	3.65	116.36	110.43
2	D	1	AOM	C7-C8-C9	3.76	114.95	110.46
2	D	1	AOM	C9-C8-C14	4.03	114.35	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	AOM	C15-C14-C13	4.03	109.06	103.82
2	C	1	AOM	C12-C13-C17	4.08	121.39	115.31
2	D	1	AOM	C16-C17-C13	4.24	107.88	104.58
2	C	1	AOM	C7-C8-C9	4.37	115.69	110.46
2	C	1	AOM	C9-C8-C14	4.79	115.34	109.06
3	F	360	NAP	O2B-P2B-O1X	4.94	119.44	107.11
3	E	360	NAP	O2B-P2B-O1X	4.94	119.45	107.11
2	D	1	AOM	C12-C13-C17	5.22	123.09	115.31
2	C	1	AOM	C16-C17-C13	6.66	109.75	104.58
3	F	360	NAP	O4D-C1D-N1N	10.60	119.77	108.13
3	E	360	NAP	O4D-C1D-N1N	10.61	119.78	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	AOM	6	0
2	D	1	AOM	15	0
3	E	360	NAP	42	0
3	F	360	NAP	24	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	278/327 (85%)	-0.11	6 (2%)	65	73	13, 30, 45, 83	13 (4%)
1	B	272/327 (83%)	-0.01	7 (2%)	59	68	14, 32, 52, 82	10 (3%)
All	All	550/654 (84%)	-0.06	13 (2%)	62	71	13, 30, 50, 83	23 (4%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	ASP	7.1
1	A	190[A]	THR	7.1
1	A	191[A]	ALA	6.4
1	A	198[A]	GLY	4.7
1	B	212	PHE	3.9
1	B	1	ALA	3.5
1	B	226	PHE	2.9
1	B	204	LEU	2.5
1	A	199	SER	2.5
1	B	57	GLY	2.4
1	B	281	ARG	2.2
1	A	202	GLU	2.1
1	A	226	PHE	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.

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6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	AOM	C	1	21/21	0.73	0.44	9.56	12,27,34,39	21
3	NAP	F	360	48/48	0.61	0.46	7.75	17,30,33,34	48
3	NAP	E	360	48/48	0.68	0.46	7.41	17,30,33,34	48
2	AOM	D	1	21/21	0.68	0.46	6.99	34,37,41,43	21

6.5 Other polymers (i)

There are no such residues in this entry.