Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:30 AM GMT

PDB ID	:	3EY4
Title	:	Further studies with the 2-amino-1,3-thiazol-4(5H)-one class of 11-hydroxysteroid dehydrogenase type 1 (11-HSD1) inhibitors: Reducing pregnane X receptor (PXR) activity and exploring activity in a monkey pharmacodynamic model
Authors	:	Zhang, J.D.; Jordan, S.R.; Li, V.
Deposited on	:	2008-10-17
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

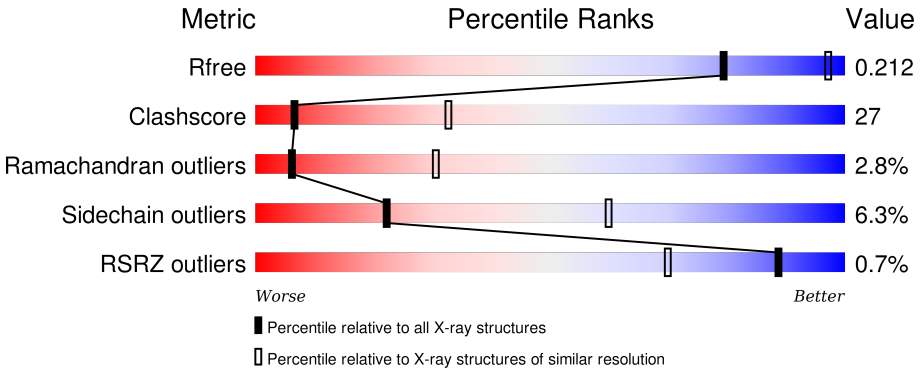
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	275	2% 39% 49% 7% 6%
1	B	275	47% 41% • 7%
1	C	275	52% 37% • 7%
1	D	275	% 47% 43% 5% 5%

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	NDP	C	503	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8171 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 11-beta-Hydroxysteroid Dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1982	1264	335	368	15			
1	B	255	Total	C	N	O	S	0	0	0
			1951	1247	331	358	15			
1	C	256	Total	C	N	O	S	0	0	0
			1960	1252	332	361	15			
1	D	261	Total	C	N	O	S	0	0	0
			2002	1277	338	372	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	EXPRESSION TAG	UNP P28845
A	19	HIS	-	EXPRESSION TAG	UNP P28845
A	20	HIS	-	EXPRESSION TAG	UNP P28845
A	21	HIS	-	EXPRESSION TAG	UNP P28845
A	22	HIS	-	EXPRESSION TAG	UNP P28845
A	23	HIS	-	EXPRESSION TAG	UNP P28845
A	24	HIS	-	EXPRESSION TAG	UNP P28845
A	272	SER	CYS	ENGINEERED	UNP P28845
B	18	MET	-	EXPRESSION TAG	UNP P28845
B	19	HIS	-	EXPRESSION TAG	UNP P28845
B	20	HIS	-	EXPRESSION TAG	UNP P28845
B	21	HIS	-	EXPRESSION TAG	UNP P28845
B	22	HIS	-	EXPRESSION TAG	UNP P28845
B	23	HIS	-	EXPRESSION TAG	UNP P28845
B	24	HIS	-	EXPRESSION TAG	UNP P28845
B	272	SER	CYS	ENGINEERED	UNP P28845
C	18	MET	-	EXPRESSION TAG	UNP P28845
C	19	HIS	-	EXPRESSION TAG	UNP P28845
C	20	HIS	-	EXPRESSION TAG	UNP P28845
C	21	HIS	-	EXPRESSION TAG	UNP P28845
C	22	HIS	-	EXPRESSION TAG	UNP P28845

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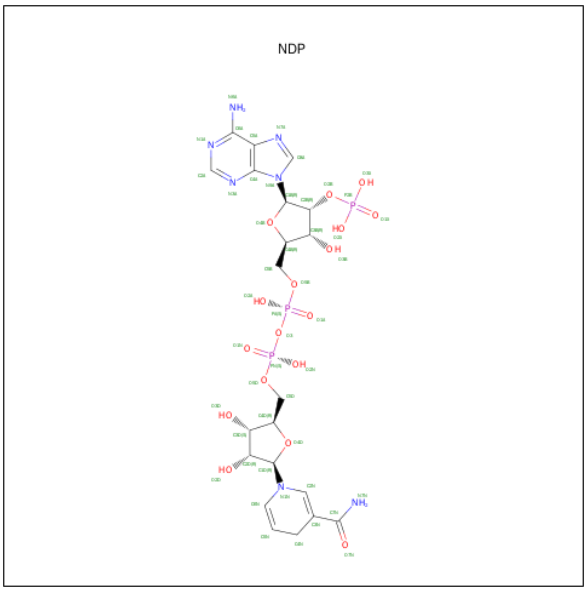
Chain	Residue	Modelled	Actual	Comment	Reference
C	23	HIS	-	EXPRESSION TAG	UNP P28845
C	24	HIS	-	EXPRESSION TAG	UNP P28845
C	272	SER	CYS	ENGINEERED	UNP P28845
D	18	MET	-	EXPRESSION TAG	UNP P28845
D	19	HIS	-	EXPRESSION TAG	UNP P28845
D	20	HIS	-	EXPRESSION TAG	UNP P28845
D	21	HIS	-	EXPRESSION TAG	UNP P28845
D	22	HIS	-	EXPRESSION TAG	UNP P28845
D	23	HIS	-	EXPRESSION TAG	UNP P28845
D	24	HIS	-	EXPRESSION TAG	UNP P28845
D	272	SER	CYS	ENGINEERED	UNP P28845

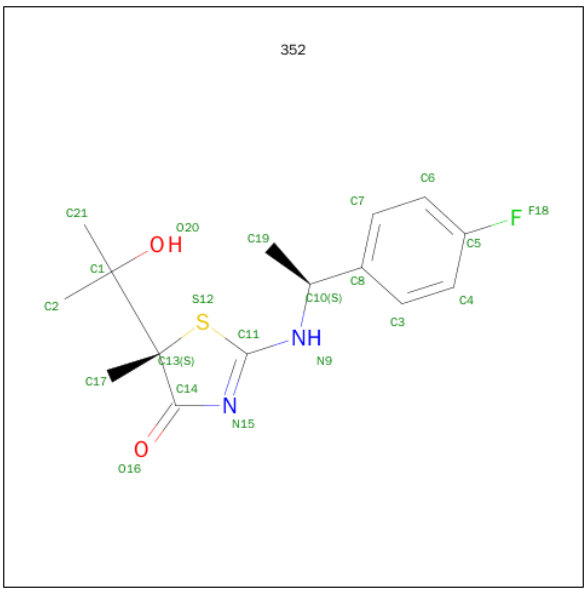
- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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-(4-FLUOROPHENYL)ETHYL]AMINO}-5-(1-HYDROXY-1-METHYLETHYL)-5-METHYL-1,3-THIAZOL-4(5H)-ONE (three-letter code: 352)

(formula: $C_{15}H_{19}FN_2O_2S$).



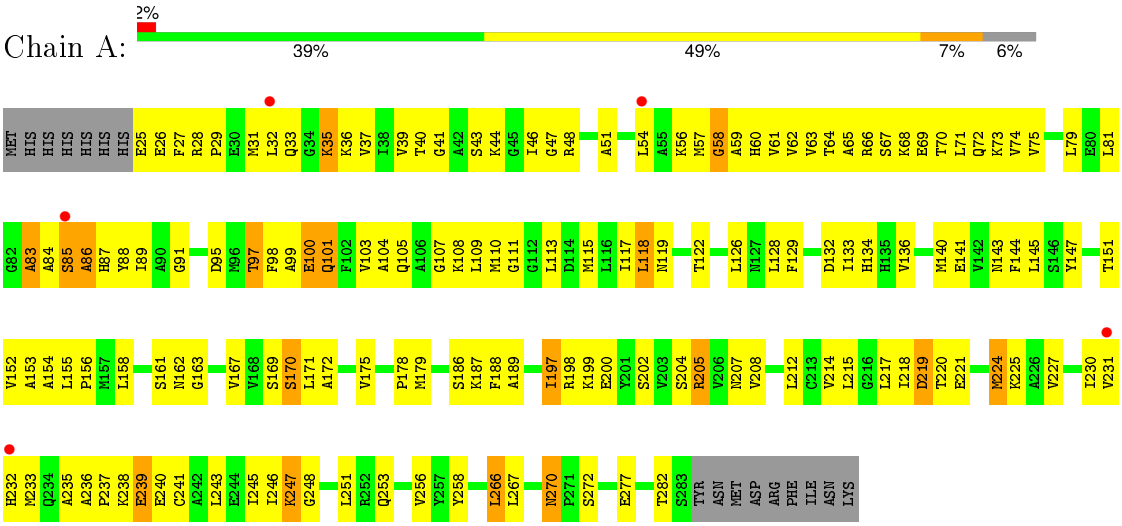
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			21	15	1	2	2	1		
3	C	1	Total	C	F	N	O	S	0	0
			21	15	1	2	2	1		
3	B	1	Total	C	F	N	O	S	0	0
			21	15	1	2	2	1		
3	D	1	Total	C	F	N	O	S	0	0
			21	15	1	2	2	1		

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.

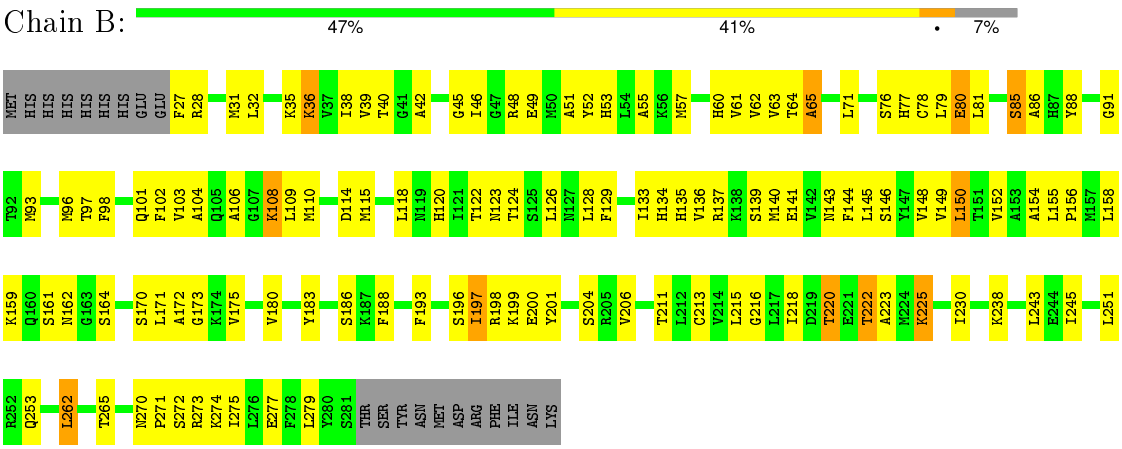
- Molecule 1: 11-beta-Hydroxysteroid Dehydrogenase 1

Chain A:



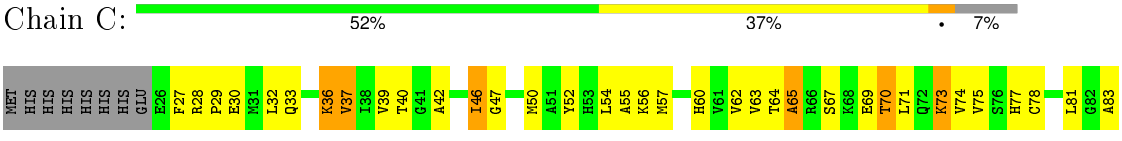
- Molecule 1: 11-beta-Hydroxysteroid Dehydrogenase 1

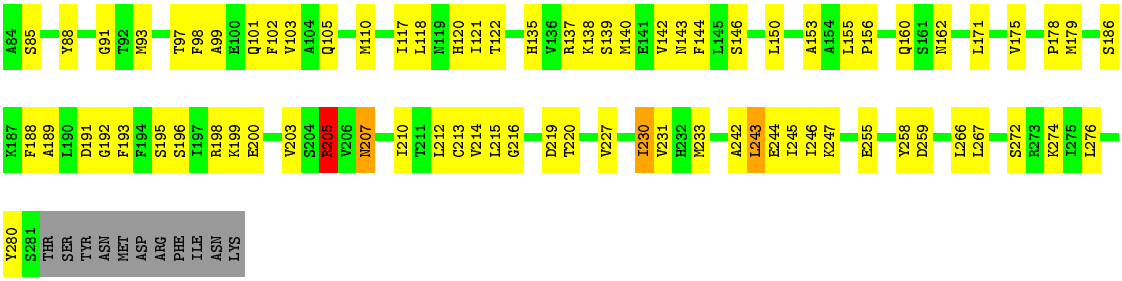
Chain B:



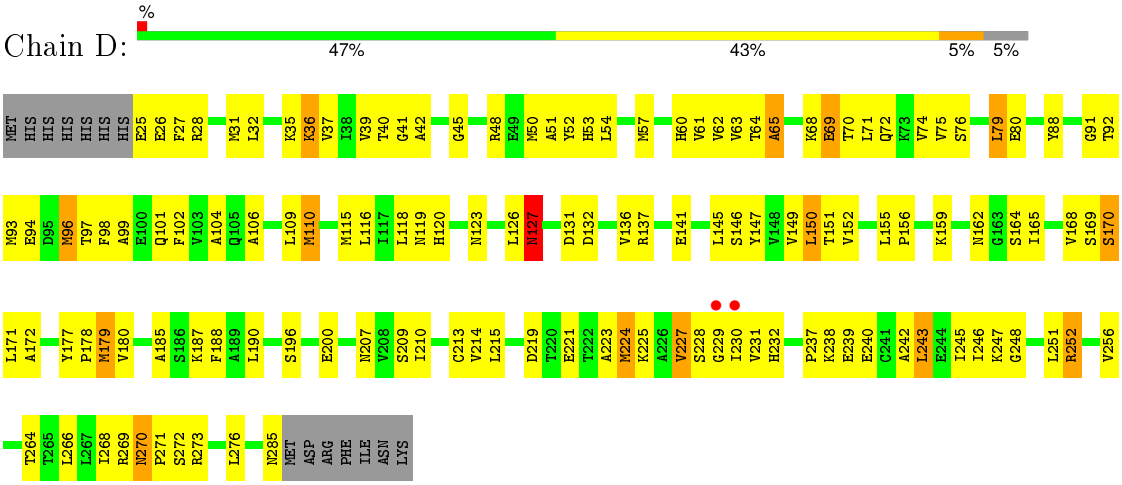
- Molecule 1: 11-beta-Hydroxysteroid Dehydrogenase 1

Chain C:





• Molecule 1: 11-beta-Hydroxysteroid Dehydrogenase 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.04Å 138.48Å 155.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 48.50 – 2.85	Depositor EDS
% Data completeness (in resolution range)	94.0 (50.00-3.00) 95.7 (48.50-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.86Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.219 , 0.319 0.233 , 0.212	Depositor DCC
R_{free} test set	1104 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 24571 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8171	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: NDP, 352

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	0.39	0/2015	0.62	0/2720
1	B	0.43	0/1984	0.64	0/2678
1	C	0.46	0/1993	0.65	0/2690
1	D	0.47	0/2036	0.68	0/2749
All	All	0.44	0/8028	0.65	0/10837

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1982	0	2031	155	0
1	B	1951	0	2007	109	0
1	C	1960	0	2013	91	0
1	D	2002	0	2046	118	0
2	A	48	0	26	5	0
2	B	48	0	26	5	0
2	C	48	0	25	3	0
2	D	48	0	26	3	0
3	A	21	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	19	3	0
3	C	21	0	19	0	0
3	D	21	0	19	2	0
All	All	8171	0	8276	447	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 27.

All (447) 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:C:243:LEU:HD13	1:C:247:LYS:HD2	1.41	0.99
1:A:129:PHE:HB3	1:B:197:ILE:HD11	1.47	0.97
1:B:46:ILE:HD11	1:B:218:ILE:HG21	1.53	0.91
1:A:29:PRO:HA	1:A:57:MET:HE3	1.56	0.87
1:A:200:GLU:HB3	1:B:128:LEU:HD22	1.56	0.86
1:A:118:LEU:H	1:A:118:LEU:HD12	1.39	0.86
1:D:40:THR:HB	1:D:120:HIS:HD2	1.39	0.86
1:A:37:VAL:HG13	1:A:61:VAL:HG12	1.55	0.86
1:A:251:LEU:HD12	1:A:253:GLN:HE21	1.38	0.86
1:D:242:ALA:O	1:D:246:ILE:HG12	1.79	0.82
1:A:60:HIS:HA	1:A:85:SER:HB3	1.63	0.81
1:A:158:LEU:HD22	1:A:163:GLY:HA3	1.63	0.80
1:D:92:THR:HB	1:D:94:GLU:HG3	1.64	0.80
1:B:220:THR:HA	1:B:238:LYS:HE2	1.62	0.80
1:C:213:CYS:SG	1:C:245:ILE:HG23	2.23	0.78
1:B:108:LYS:HE2	1:B:108:LYS:N	1.98	0.78
1:A:197:ILE:HD11	1:B:129:PHE:HB3	1.64	0.78
1:C:175:VAL:HG12	1:D:273:ARG:HG3	1.67	0.76
1:B:155:LEU:HG	1:B:159:LYS:HE3	1.69	0.75
1:D:40:THR:CB	1:D:120:HIS:HD2	1.99	0.74
1:B:60:HIS:HB3	1:B:110:MET:HE2	1.68	0.74
1:A:113:LEU:HD23	1:A:154:ALA:HB1	1.68	0.74
1:B:215:LEU:HD21	1:B:245:ILE:HD11	1.70	0.74
1:B:225:LYS:HB2	1:B:225:LYS:HZ3	1.53	0.74
1:C:28:ARG:HG2	1:C:28:ARG:HH11	1.51	0.73
1:C:146:SER:O	1:C:150:LEU:HB2	1.88	0.73
1:A:46:ILE:HD11	1:A:218:ILE:HG21	1.70	0.72
1:B:104:ALA:O	1:B:108:LYS:HD2	1.89	0.72
1:C:267:LEU:HB2	1:D:276:LEU:HD13	1.72	0.72
1:A:220:THR:HG21	2:A:501:NDP:O1N	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LEU:HD22	1:B:200:GLU:HB3	1.70	0.71
1:A:28:ARG:HB2	1:A:31:MET:HG3	1.73	0.71
1:D:230:ILE:HD12	1:D:230:ILE:H	1.54	0.71
1:A:175:VAL:HG22	1:B:273:ARG:HG3	1.73	0.70
1:D:37:VAL:HG22	1:D:115:MET:HB3	1.73	0.70
1:B:42:ALA:HB3	1:B:63:VAL:HB	1.73	0.70
1:D:40:THR:HB	1:D:120:HIS:CD2	2.25	0.70
1:B:60:HIS:ND1	1:B:85:SER:HB3	2.06	0.69
1:B:139:SER:O	1:B:143:ASN:HB2	1.92	0.69
1:A:162:ASN:HD22	1:A:207:ASN:HD22	1.40	0.69
1:A:126:LEU:HD13	1:A:231:VAL:HG23	1.73	0.69
1:C:230:ILE:N	1:C:230:ILE:HD12	2.09	0.68
1:D:40:THR:HG1	1:D:119:ASN:H	1.42	0.68
1:A:32:LEU:HA	1:A:35:LYS:HD3	1.75	0.68
1:B:213:CYS:SG	1:B:245:ILE:HG23	2.33	0.68
1:B:225:LYS:HB2	1:B:225:LYS:NZ	2.09	0.68
1:C:37:VAL:HG21	1:C:54:LEU:HD13	1.76	0.68
1:D:227:VAL:HG12	1:D:228:SER:H	1.60	0.67
1:C:205:ARG:NE	1:C:205:ARG:O	2.27	0.67
1:C:216:GLY:HA3	1:C:259:ASP:OD1	1.94	0.67
1:C:93:MET:HG3	1:C:120:HIS:CD2	2.29	0.67
1:A:227:VAL:HG13	1:A:231:VAL:HB	1.77	0.67
1:D:177:TYR:CD2	3:D:604:352:H2	2.30	0.67
1:A:108:LYS:HE3	1:C:97:THR:HA	1.77	0.67
1:C:64:THR:HB	1:C:102:PHE:CE1	2.30	0.67
1:C:212:LEU:HD23	1:C:255:GLU:OE2	1.95	0.66
1:A:162:ASN:ND2	1:A:207:ASN:HD22	1.94	0.66
1:C:67:SER:HB2	1:C:70:THR:HG23	1.78	0.66
1:D:75:VAL:O	1:D:79:LEU:HD22	1.96	0.65
1:D:61:VAL:C	1:D:110:MET:HE1	2.16	0.65
1:D:231:VAL:HG12	1:D:232:HIS:H	1.62	0.65
1:D:68:LYS:O	1:D:72:GLN:HG3	1.97	0.65
1:C:60:HIS:ND1	1:C:85:SER:HB2	2.11	0.65
1:C:276:LEU:HD12	1:C:276:LEU:O	1.97	0.65
1:A:97:THR:HA	1:A:100:GLU:HB2	1.78	0.64
1:A:43:SER:HB3	2:A:501:NDP:O3B	1.97	0.64
1:D:231:VAL:HG12	1:D:232:HIS:N	2.13	0.64
1:A:248:GLY:HA3	1:A:256:VAL:HG21	1.78	0.64
1:C:137:ARG:HH22	1:D:96:MET:HG3	1.63	0.64
1:A:32:LEU:HD23	1:A:35:LYS:HG3	1.79	0.63
1:A:140:MET:HG3	1:B:144:PHE:CE2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:MET:HG3	1:B:144:PHE:HE2	1.63	0.63
1:C:244:GLU:HG3	1:C:258:TYR:CE2	2.34	0.63
1:C:62:VAL:HG23	1:C:110:MET:SD	2.38	0.63
1:C:267:LEU:CB	1:D:276:LEU:HD13	2.28	0.63
1:C:220:THR:HG21	2:C:503:NDP:O2N	1.97	0.63
1:A:69:GLU:HA	1:A:72:GLN:HB3	1.81	0.62
1:B:124:THR:HG22	1:B:135:HIS:HE1	1.64	0.62
1:A:28:ARG:HG3	1:A:28:ARG:HH11	1.64	0.62
1:A:236:ALA:HB1	1:A:237:PRO:HD2	1.81	0.61
1:D:28:ARG:HB2	1:D:31:MET:HG3	1.82	0.61
1:A:39:VAL:HG22	1:A:117:ILE:HD12	1.82	0.61
1:A:56:LYS:CG	1:A:81:LEU:HB3	2.31	0.60
1:C:199:LYS:O	1:C:203:VAL:HG23	2.01	0.60
1:B:28:ARG:O	1:B:31:MET:HG3	2.01	0.60
1:A:32:LEU:HD13	1:A:54:LEU:CD2	2.31	0.60
1:C:230:ILE:H	1:C:230:ILE:HD12	1.66	0.60
1:D:126:LEU:O	1:D:127:ASN:HB2	2.00	0.60
1:A:32:LEU:HA	1:A:35:LYS:CD	2.31	0.60
1:D:40:THR:HA	1:D:64:THR:HG22	1.82	0.60
1:A:129:PHE:CB	1:B:197:ILE:HD11	2.29	0.60
1:C:69:GLU:O	1:C:73:LYS:HD2	2.01	0.60
1:D:225:LYS:HB2	1:D:225:LYS:NZ	2.17	0.59
1:A:155:LEU:HB3	1:A:156:PRO:HD3	1.84	0.59
1:C:99:ALA:HB1	1:C:150:LEU:HD13	1.84	0.59
1:D:223:ALA:O	1:D:227:VAL:HG23	2.02	0.59
1:A:251:LEU:HD12	1:A:253:GLN:NE2	2.14	0.59
1:C:46:ILE:O	1:C:50:MET:HG3	2.02	0.58
1:A:32:LEU:CD2	1:A:35:LYS:HG3	2.33	0.58
1:B:27:PHE:HB2	1:B:251:LEU:HD21	1.86	0.58
1:A:67:SER:CB	1:A:70:THR:HB	2.33	0.58
1:B:40:THR:CB	1:B:120:HIS:HD2	2.17	0.58
1:B:135:HIS:HB2	1:D:97:THR:HG21	1.85	0.58
1:C:93:MET:HG3	1:C:120:HIS:NE2	2.18	0.58
1:C:103:VAL:HG21	1:C:153:ALA:HB3	1.85	0.58
1:D:171:LEU:HD23	1:D:214:VAL:HG12	1.86	0.57
1:A:67:SER:HB3	1:A:70:THR:OG1	2.04	0.57
1:C:42:ALA:HB3	1:C:63:VAL:HB	1.84	0.57
1:C:101:GLN:HB3	1:C:105:GLN:HE22	1.70	0.57
1:D:227:VAL:HG12	1:D:228:SER:N	2.19	0.57
1:B:171:LEU:HG	1:B:216:GLY:HA2	1.87	0.57
1:A:161:SER:O	1:A:162:ASN:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LYS:HG3	1:C:110:MET:HB3	1.85	0.57
1:A:37:VAL:HG11	1:A:54:LEU:HD13	1.86	0.57
1:C:139:SER:O	1:C:143:ASN:HB2	2.05	0.57
1:B:77:HIS:O	1:B:80:GLU:HG2	2.05	0.57
1:C:227:VAL:HG13	1:C:231:VAL:HB	1.86	0.56
1:B:155:LEU:CG	1:B:159:LYS:HE3	2.35	0.56
1:C:37:VAL:HG21	1:C:54:LEU:CD1	2.34	0.56
1:A:56:LYS:HG2	1:A:81:LEU:HB3	1.88	0.56
1:A:132:ASP:O	1:A:136:VAL:HG23	2.05	0.56
1:A:63:VAL:O	1:A:88:TYR:HA	2.05	0.56
1:A:99:ALA:O	1:A:103:VAL:HG23	2.06	0.56
1:B:62:VAL:HG23	1:B:110:MET:CE	2.36	0.56
1:D:155:LEU:CD2	1:D:159:LYS:HE3	2.36	0.56
1:D:270:ASN:HD21	1:D:272:SER:HB2	1.68	0.56
1:D:165:ILE:HD12	1:D:210:ILE:HG12	1.88	0.56
1:A:167:VAL:HG23	1:A:212:LEU:HD12	1.87	0.56
1:A:101:GLN:O	1:A:105:GLN:HG2	2.05	0.56
1:D:60:HIS:HB3	1:D:110:MET:HE2	1.87	0.55
1:C:171:LEU:HD23	1:C:214:VAL:HG12	1.88	0.55
1:C:171:LEU:HG	1:C:215:LEU:O	2.06	0.55
1:D:71:LEU:O	1:D:74:VAL:HG12	2.06	0.55
1:A:247:LYS:NZ	1:A:251:LEU:HD11	2.22	0.55
1:A:36:LYS:HE3	1:A:111:GLY:O	2.07	0.55
1:A:97:THR:O	1:A:100:GLU:HB2	2.07	0.55
1:C:122:THR:HB	1:C:142:VAL:HG11	1.88	0.55
1:A:126:LEU:HD11	1:A:227:VAL:HG22	1.89	0.55
1:A:104:ALA:O	1:A:108:LYS:HG2	2.07	0.55
1:D:106:ALA:HA	1:D:109:LEU:HD12	1.88	0.55
1:A:67:SER:HB3	1:A:70:THR:CB	2.37	0.55
1:C:32:LEU:HD13	1:C:54:LEU:CD2	2.37	0.55
1:B:93:MET:HG3	1:B:120:HIS:CE1	2.42	0.55
1:C:28:ARG:HG2	1:C:28:ARG:NH1	2.20	0.54
1:C:32:LEU:HD13	1:C:54:LEU:HD23	1.89	0.54
1:B:124:THR:HG22	1:B:135:HIS:CE1	2.43	0.54
1:C:40:THR:HA	1:C:64:THR:HG23	1.89	0.54
1:B:64:THR:O	1:B:65:ALA:HB2	2.08	0.54
1:D:168:VAL:HA	1:D:213:CYS:HB2	1.90	0.54
1:D:172:ALA:O	1:D:188:PHE:HE1	1.91	0.54
1:B:262:LEU:H	1:B:262:LEU:HD12	1.73	0.54
1:D:101:GLN:O	1:D:104:ALA:HB3	2.08	0.54
1:D:126:LEU:HD12	1:D:126:LEU:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:PRO:O	1:D:159:LYS:HB2	2.08	0.54
1:B:77:HIS:O	1:B:81:LEU:HG	2.07	0.54
1:C:103:VAL:HG21	1:C:153:ALA:CB	2.38	0.54
1:A:237:PRO:HG2	1:A:258:TYR:OH	2.09	0.53
1:C:73:LYS:H	1:C:73:LYS:HD2	1.74	0.53
1:D:123:ASN:N	1:D:123:ASN:HD22	2.05	0.53
1:D:187:LYS:HE3	2:D:504:NDP:O2D	2.08	0.53
1:C:60:HIS:ND1	1:C:85:SER:CB	2.72	0.53
1:B:222:THR:HB	2:B:502:NDP:O2A	2.08	0.53
1:A:239:GLU:HG3	1:A:240:GLU:N	2.23	0.53
1:A:270:ASN:HD22	1:A:270:ASN:C	2.10	0.53
1:D:215:LEU:HD21	1:D:245:ILE:HD11	1.90	0.53
1:B:48:ARG:O	1:B:51:ALA:HB3	2.09	0.53
1:D:96:MET:SD	1:D:149:VAL:HG21	2.48	0.53
1:C:101:GLN:HB3	1:C:105:GLN:NE2	2.24	0.53
1:A:32:LEU:HD13	1:A:54:LEU:HD23	1.90	0.53
1:D:145:LEU:O	1:D:149:VAL:HG23	2.09	0.53
1:D:219:ASP:OD1	1:D:238:LYS:N	2.42	0.53
1:B:97:THR:O	1:B:101:GLN:HG3	2.09	0.53
1:B:35:LYS:HD2	1:B:114:ASP:CG	2.29	0.52
1:B:148:VAL:O	1:B:152:VAL:HG23	2.08	0.52
1:D:63:VAL:O	1:D:88:TYR:HA	2.09	0.52
1:C:65:ALA:HB3	1:C:71:LEU:HD21	1.91	0.52
1:B:140:MET:SD	1:B:186:SER:HA	2.50	0.52
1:A:67:SER:HB3	1:A:70:THR:HB	1.92	0.52
1:B:122:THR:O	1:B:124:THR:HG23	2.10	0.52
1:A:133:ILE:HA	1:A:136:VAL:CG2	2.40	0.52
1:A:171:LEU:HD23	1:A:214:VAL:HG12	1.92	0.52
1:A:32:LEU:HA	1:A:35:LYS:CG	2.40	0.52
1:D:48:ARG:HG3	1:D:74:VAL:HG23	1.92	0.52
1:A:133:ILE:HA	1:A:136:VAL:HG23	1.92	0.51
1:A:172:ALA:O	1:A:188:PHE:HE1	1.92	0.51
1:D:32:LEU:HD23	1:D:54:LEU:CD2	2.40	0.51
1:A:75:VAL:HG13	1:A:86:ALA:HB1	1.91	0.51
1:D:62:VAL:HG23	1:D:110:MET:HE3	1.91	0.51
1:D:164:SER:HB3	1:D:209:SER:OG	2.10	0.51
1:B:126:LEU:HD12	1:B:230:ILE:HD12	1.92	0.51
1:C:205:ARG:C	1:C:205:ARG:HE	2.14	0.51
1:C:171:LEU:CD1	1:C:216:GLY:HA2	2.41	0.51
1:B:40:THR:HA	1:B:64:THR:CG2	2.41	0.51
1:C:266:LEU:O	1:C:266:LEU:HD12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ARG:O	1:D:31:MET:HG3	2.10	0.51
1:D:32:LEU:HA	1:D:35:LYS:HG3	1.93	0.51
1:B:146:SER:O	1:B:150:LEU:HD22	2.11	0.51
1:A:36:LYS:HD3	1:A:110:MET:HB3	1.92	0.51
1:B:155:LEU:O	1:B:158:LEU:N	2.42	0.51
1:A:37:VAL:O	1:A:61:VAL:HA	2.11	0.51
1:D:120:HIS:HE1	1:D:146:SER:OG	1.94	0.51
1:C:30:GLU:CD	1:C:30:GLU:H	2.14	0.51
1:A:197:ILE:HD11	1:B:129:PHE:CB	2.37	0.50
1:A:56:LYS:HG3	1:A:81:LEU:HB3	1.93	0.50
1:D:64:THR:HB	1:D:102:PHE:CZ	2.46	0.50
1:B:40:THR:HA	1:B:64:THR:HG22	1.93	0.50
1:D:62:VAL:HG23	1:D:110:MET:CE	2.41	0.50
1:A:37:VAL:HG11	1:A:54:LEU:HD22	1.94	0.50
1:B:225:LYS:CB	1:B:225:LYS:NZ	2.74	0.50
1:A:178:PRO:O	1:A:179:MET:HB2	2.11	0.50
1:D:137:ARG:HG3	1:D:137:ARG:HH11	1.77	0.50
1:D:238:LYS:NZ	1:D:239:GLU:OE2	2.40	0.50
1:D:93:MET:HG3	1:D:120:HIS:CE1	2.46	0.50
1:A:105:GLN:O	1:A:109:LEU:HB2	2.12	0.50
1:A:37:VAL:CG1	1:A:61:VAL:HG12	2.37	0.50
1:C:118:LEU:HD22	1:C:150:LEU:HD23	1.92	0.50
1:A:240:GLU:HB3	1:A:258:TYR:OH	2.11	0.50
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.95	0.50
1:C:39:VAL:HG12	1:C:42:ALA:HB2	1.94	0.50
1:D:52:TYR:CE1	1:D:74:VAL:HG23	2.46	0.50
1:D:243:LEU:HD22	1:D:247:LYS:HE3	1.94	0.50
1:D:248:GLY:HA3	1:D:256:VAL:HG21	1.94	0.50
1:A:35:LYS:H	1:A:35:LYS:CD	2.24	0.50
1:D:62:VAL:HG11	1:D:106:ALA:CB	2.42	0.49
1:D:91:GLY:HA3	1:D:98:PHE:CE2	2.46	0.49
1:C:242:ALA:O	1:C:246:ILE:HG13	2.11	0.49
1:A:32:LEU:HB2	1:A:57:MET:HE2	1.93	0.49
1:D:123:ASN:N	1:D:123:ASN:ND2	2.58	0.49
1:A:197:ILE:HG22	1:A:198:ARG:N	2.28	0.49
1:C:200:GLU:OE1	1:D:179:MET:N	2.45	0.49
1:A:79:LEU:HA	1:A:83:ALA:HB3	1.94	0.49
1:A:158:LEU:CD2	1:A:163:GLY:HA3	2.38	0.49
1:D:62:VAL:HG11	1:D:106:ALA:HB2	1.95	0.49
1:A:107:GLY:C	1:A:109:LEU:H	2.14	0.49
1:A:227:VAL:HG12	1:A:227:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:SER:HB2	1:A:70:THR:HB	1.93	0.49
1:A:103:VAL:HG21	1:A:153:ALA:HB3	1.95	0.49
1:A:199:LYS:O	1:A:202:SER:HB3	2.12	0.49
1:A:48:ARG:O	1:A:51:ALA:HB3	2.12	0.49
1:A:100:GLU:HA	1:A:100:GLU:OE1	2.13	0.49
1:A:238:LYS:HG3	1:A:239:GLU:N	2.27	0.49
1:A:241:CYS:HB2	1:A:258:TYR:CE1	2.48	0.49
2:B:502:NDP:H41N	3:B:603:352:C11	2.43	0.49
1:A:145:LEU:HD21	1:B:137:ARG:HD3	1.95	0.49
1:C:91:GLY:HA3	1:C:98:PHE:CZ	2.48	0.48
1:D:132:ASP:O	1:D:136:VAL:HG23	2.13	0.48
1:B:172:ALA:O	1:B:188:PHE:HE1	1.96	0.48
1:C:55:ALA:HB2	1:C:78:CYS:SG	2.54	0.48
1:A:44:LYS:HG2	2:A:501:NDP:H3B	1.94	0.48
1:B:62:VAL:HG23	1:B:110:MET:HE3	1.96	0.48
1:D:123:ASN:ND2	1:D:123:ASN:H	2.12	0.48
1:B:133:ILE:HA	1:B:136:VAL:HB	1.95	0.48
1:B:40:THR:HB	1:B:120:HIS:CD2	2.49	0.48
1:C:75:VAL:HG21	1:C:88:TYR:HB3	1.96	0.48
1:C:243:LEU:O	1:C:247:LYS:HG3	2.13	0.48
1:C:198:ARG:HA	1:C:210:ILE:HD12	1.96	0.48
1:D:266:LEU:O	1:D:269:ARG:HG2	2.14	0.47
1:A:37:VAL:CG1	1:A:54:LEU:HD13	2.44	0.47
1:C:191:ASP:O	1:C:195:SER:HB2	2.15	0.47
1:B:32:LEU:HD23	1:B:57:MET:HE1	1.96	0.47
1:A:204:SER:O	1:A:205:ARG:HG2	2.13	0.47
1:A:71:LEU:O	1:A:74:VAL:HG22	2.14	0.47
1:B:91:GLY:HA3	1:B:98:PHE:CZ	2.49	0.47
1:B:61:VAL:O	1:B:86:ALA:HA	2.14	0.47
1:B:155:LEU:O	1:B:156:PRO:C	2.53	0.47
1:C:32:LEU:HD11	1:C:246:ILE:CG2	2.45	0.47
1:C:67:SER:OG	2:C:503:NDP:O2X	2.23	0.47
1:B:64:THR:HB	1:B:102:PHE:CZ	2.49	0.47
1:D:238:LYS:HG3	1:D:239:GLU:OE2	2.15	0.47
1:C:244:GLU:HG3	1:C:258:TYR:CD2	2.50	0.47
1:D:27:PHE:HB2	1:D:251:LEU:HD11	1.96	0.47
1:B:155:LEU:CD2	1:B:159:LYS:HE3	2.45	0.47
1:A:41:GLY:O	1:A:47:GLY:HA3	2.15	0.47
1:B:52:TYR:O	1:B:55:ALA:HB3	2.15	0.47
1:B:36:LYS:HB3	1:B:110:MET:SD	2.55	0.47
1:A:175:VAL:HG13	1:B:277:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ILE:N	1:C:230:ILE:CD1	2.77	0.47
1:B:134:HIS:CD2	1:B:137:ARG:HH22	2.33	0.46
1:D:36:LYS:HD2	1:D:36:LYS:N	2.29	0.46
1:C:75:VAL:CG2	1:C:88:TYR:HB3	2.44	0.46
1:A:175:VAL:HG13	1:B:277:GLU:CG	2.45	0.46
1:C:230:ILE:H	1:C:230:ILE:CD1	2.28	0.46
1:A:95:ASP:CG	1:A:97:THR:HG23	2.36	0.46
1:B:40:THR:HB	1:B:120:HIS:HD2	1.81	0.46
1:D:224:MET:N	1:D:224:MET:SD	2.89	0.46
1:A:35:LYS:H	1:A:35:LYS:HD2	1.81	0.46
1:C:77:HIS:CE1	1:C:81:LEU:HG	2.51	0.46
1:A:32:LEU:HD13	1:A:54:LEU:HD21	1.98	0.46
1:B:197:ILE:HA	1:B:197:ILE:HD13	1.64	0.46
1:D:61:VAL:CA	1:D:110:MET:HE1	2.45	0.46
1:A:26:GLU:CD	1:A:27:PHE:N	2.69	0.46
1:D:237:PRO:HB2	1:D:240:GLU:HB3	1.98	0.46
1:A:217:LEU:HG	1:A:235:ALA:HB2	1.98	0.46
1:C:192:GLY:O	1:C:196:SER:HB2	2.16	0.45
1:B:275:ILE:O	1:B:279:LEU:HG	2.16	0.45
1:C:186:SER:O	1:C:189:ALA:HB3	2.15	0.45
1:B:180:VAL:HB	1:B:183:TYR:HB3	1.98	0.45
1:D:227:VAL:CG1	1:D:228:SER:H	2.24	0.45
1:A:87:HIS:NE2	1:A:109:LEU:HD21	2.31	0.45
1:B:141:GLU:HA	1:B:145:LEU:HB2	1.97	0.45
1:D:270:ASN:C	1:D:270:ASN:ND2	2.69	0.45
1:A:171:LEU:HG	1:A:215:LEU:O	2.17	0.45
1:A:277:GLU:CG	1:B:175:VAL:HG13	2.46	0.45
1:D:155:LEU:HG	1:D:159:LYS:HG3	1.99	0.45
1:D:271:PRO:O	1:D:272:SER:C	2.55	0.45
1:A:172:ALA:O	1:A:188:PHE:CE1	2.69	0.45
1:A:85:SER:O	1:A:86:ALA:HB2	2.16	0.45
1:B:64:THR:HB	1:B:102:PHE:CE1	2.51	0.45
1:A:95:ASP:OD2	1:A:97:THR:HG23	2.16	0.45
1:A:89:ILE:HD13	1:A:105:GLN:HG3	1.98	0.45
1:C:155:LEU:HB3	1:C:156:PRO:HD3	1.99	0.45
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.68	0.45
1:B:204:SER:HB2	1:B:206:VAL:HG23	1.98	0.45
1:A:97:THR:CA	1:A:100:GLU:HB2	2.46	0.45
1:B:115:MET:HG2	1:B:164:SER:OG	2.16	0.45
1:C:52:TYR:O	1:C:56:LYS:HG3	2.17	0.45
1:A:32:LEU:HD12	1:A:57:MET:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:SER:O	1:D:80:GLU:HG3	2.17	0.45
1:D:116:LEU:HD21	1:D:118:LEU:HD21	1.99	0.45
1:D:145:LEU:HA	1:D:145:LEU:HD23	1.67	0.45
1:A:232:HIS:O	1:A:233:MET:HB2	2.17	0.45
1:D:177:TYR:HD1	1:D:178:PRO:O	2.01	0.44
1:B:183:TYR:CZ	3:B:603:352:H19B	2.51	0.44
1:D:251:LEU:O	1:D:252:ARG:HB2	2.17	0.44
1:D:99:ALA:HB1	1:D:150:LEU:HD13	1.99	0.44
1:B:106:ALA:HA	1:B:109:LEU:HD12	1.99	0.44
1:D:137:ARG:NH1	1:D:137:ARG:HG3	2.32	0.44
1:A:144:PHE:O	1:A:147:TYR:HB2	2.17	0.44
1:A:109:LEU:HD23	1:A:109:LEU:O	2.17	0.44
1:C:150:LEU:HD12	1:C:150:LEU:HA	1.80	0.44
1:D:25:GLU:HG3	1:D:26:GLU:OE2	2.18	0.44
1:A:200:GLU:CB	1:B:128:LEU:HD22	2.37	0.44
1:D:187:LYS:HD3	1:D:190:LEU:HD12	1.98	0.44
1:B:171:LEU:C	1:B:173:GLY:N	2.71	0.44
1:D:196:SER:O	1:D:200:GLU:HG3	2.18	0.44
1:C:71:LEU:O	1:C:74:VAL:HB	2.18	0.44
1:A:107:GLY:C	1:A:109:LEU:N	2.71	0.44
1:A:91:GLY:HA3	1:A:98:PHE:CE2	2.53	0.44
1:C:137:ARG:HH22	1:D:96:MET:CG	2.30	0.44
1:A:117:ILE:O	1:A:117:ILE:HG22	2.17	0.44
1:D:120:HIS:CE1	1:D:146:SER:OG	2.71	0.44
1:B:62:VAL:HG11	1:B:106:ALA:CB	2.48	0.44
1:C:47:GLY:O	1:C:50:MET:HB2	2.18	0.44
1:A:33:GLN:O	1:A:58:GLY:O	2.36	0.44
1:D:169:SER:OG	1:D:170:SER:N	2.48	0.44
1:B:76:SER:O	1:B:79:LEU:N	2.51	0.44
1:D:231:VAL:CG1	1:D:232:HIS:H	2.30	0.43
1:A:155:LEU:O	1:A:156:PRO:C	2.55	0.43
1:C:188:PHE:HB3	1:D:188:PHE:HB3	2.00	0.43
1:A:215:LEU:HD11	1:A:245:ILE:HD11	1.99	0.43
1:A:178:PRO:HD3	1:B:199:LYS:HD3	1.99	0.43
1:A:91:GLY:HA3	1:A:98:PHE:CZ	2.53	0.43
1:A:40:THR:HA	1:A:64:THR:HG22	2.00	0.43
1:A:69:GLU:HA	1:A:72:GLN:CB	2.47	0.43
1:D:40:THR:O	1:D:119:ASN:HB3	2.19	0.43
1:A:128:LEU:HA	1:B:200:GLU:OE2	2.18	0.43
1:B:71:LEU:HB3	1:B:88:TYR:HB2	2.00	0.43
1:D:231:VAL:CG1	1:D:232:HIS:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:SER:HB3	2:A:501:NDP:H5N	1.99	0.43
1:D:270:ASN:HD22	1:D:270:ASN:C	2.20	0.43
1:A:200:GLU:OE2	1:B:128:LEU:HA	2.19	0.43
1:B:32:LEU:HB2	1:B:57:MET:HE1	2.00	0.43
1:D:221:GLU:OE1	1:D:221:GLU:HA	2.18	0.43
1:D:155:LEU:HD23	1:D:159:LYS:HE3	2.00	0.43
1:A:167:VAL:O	1:A:167:VAL:HG23	2.18	0.43
1:B:161:SER:O	1:B:162:ASN:C	2.57	0.43
1:A:62:VAL:HG23	1:A:110:MET:SD	2.59	0.43
1:A:270:ASN:ND2	1:A:270:ASN:C	2.72	0.43
1:B:91:GLY:HA3	1:B:98:PHE:CE1	2.54	0.43
1:D:264:THR:O	1:D:268:ILE:HB	2.18	0.43
1:A:87:HIS:CD2	1:A:109:LEU:HD21	2.54	0.42
1:C:140:MET:O	1:C:144:PHE:HB3	2.19	0.42
1:B:193:PHE:O	1:B:196:SER:HB3	2.19	0.42
1:A:163:GLY:O	1:A:208:VAL:HG13	2.19	0.42
1:C:178:PRO:O	1:C:179:MET:HB2	2.18	0.42
1:B:118:LEU:HD23	1:B:118:LEU:N	2.34	0.42
1:C:27:PHE:CD2	1:C:247:LYS:HG2	2.55	0.42
1:D:32:LEU:HD22	1:D:57:MET:SD	2.60	0.42
1:D:32:LEU:HD23	1:D:54:LEU:HD23	2.02	0.42
1:C:83:ALA:HB1	1:C:85:SER:O	2.20	0.42
1:D:53:HIS:HE1	1:D:239:GLU:O	2.03	0.42
1:A:26:GLU:CD	1:A:27:PHE:H	2.23	0.42
1:B:271:PRO:HG2	1:B:272:SER:H	1.85	0.42
1:B:170:SER:HB3	2:B:502:NDP:H6N	2.00	0.42
1:C:70:THR:O	1:C:74:VAL:HG23	2.19	0.42
1:B:108:LYS:CA	1:B:108:LYS:HE2	2.49	0.42
1:B:154:ALA:O	1:B:158:LEU:HG	2.20	0.42
1:C:28:ARG:HA	1:C:29:PRO:HD3	1.92	0.42
1:A:66:ARG:HD3	2:A:501:NDP:N6A	2.35	0.42
1:D:178:PRO:O	1:D:180:VAL:HG22	2.19	0.42
1:B:216:GLY:O	2:B:502:NDP:H42N	2.20	0.42
1:D:39:VAL:HG12	1:D:42:ALA:HB2	2.00	0.42
1:A:75:VAL:HG13	1:A:86:ALA:CB	2.49	0.42
1:A:231:VAL:O	1:A:231:VAL:HG12	2.20	0.42
1:D:65:ALA:HB3	1:D:71:LEU:HD11	2.02	0.42
2:D:504:NDP:C2N	3:D:604:352:H19	2.49	0.42
1:A:113:LEU:CD2	1:A:154:ALA:HB1	2.44	0.41
1:A:219:ASP:OD1	1:A:238:LYS:N	2.53	0.41
1:D:48:ARG:HG3	1:D:74:VAL:CG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:MET:HA	1:A:224:MET:CE	2.50	0.41
1:B:96:MET:SD	1:B:149:VAL:HG21	2.60	0.41
1:A:186:SER:O	1:A:189:ALA:HB3	2.19	0.41
1:A:169:SER:HA	1:A:187:LYS:HE3	2.03	0.41
1:B:53:HIS:HD2	1:B:243:LEU:HD13	1.85	0.41
1:D:50:MET:HB3	1:D:246:ILE:HD11	2.02	0.41
1:A:247:LYS:HZ2	1:A:251:LEU:HD11	1.85	0.41
1:D:118:LEU:HD13	1:D:147:TYR:HB3	2.02	0.41
1:A:73:LYS:HB2	1:A:73:LYS:HE3	1.75	0.41
1:D:40:THR:O	1:D:41:GLY:C	2.58	0.41
1:A:247:LYS:HD3	1:A:247:LYS:C	2.40	0.41
1:A:36:LYS:HA	1:A:60:HIS:HB2	2.02	0.41
1:A:243:LEU:O	1:A:246:ILE:HB	2.21	0.41
1:D:227:VAL:C	1:D:229:GLY:H	2.23	0.41
1:D:187:LYS:CE	2:D:504:NDP:O2D	2.69	0.41
1:A:267:LEU:HD13	1:B:275:ILE:HG22	2.02	0.41
1:A:277:GLU:HG2	1:B:175:VAL:HG13	2.03	0.41
1:A:151:THR:O	1:A:152:VAL:C	2.59	0.41
1:B:198:ARG:O	1:B:201:TYR:HB2	2.20	0.41
1:C:274:LYS:HA	1:C:274:LYS:HD3	1.74	0.41
1:C:162:ASN:ND2	1:C:207:ASN:HB3	2.36	0.41
1:A:35:LYS:HD2	1:A:35:LYS:N	2.35	0.41
1:B:103:VAL:HG23	1:B:104:ALA:N	2.36	0.41
1:B:64:THR:OG1	1:B:65:ALA:N	2.54	0.41
1:C:193:PHE:HB2	1:D:185:ALA:HB2	2.03	0.41
1:A:35:LYS:O	1:A:59:ALA:HB1	2.20	0.41
1:D:50:MET:O	1:D:54:LEU:HG	2.20	0.41
1:B:64:THR:O	1:B:65:ALA:CB	2.69	0.41
1:C:231:VAL:HG12	1:C:233:MET:H	1.86	0.41
1:D:48:ARG:O	1:D:51:ALA:HB3	2.21	0.41
1:D:151:THR:O	1:D:152:VAL:C	2.59	0.41
1:D:162:ASN:HA	1:D:207:ASN:O	2.20	0.41
1:B:45:GLY:O	1:B:49:GLU:HG2	2.21	0.41
1:A:25:GLU:O	1:A:25:GLU:HG3	2.20	0.41
1:B:211:THR:HG23	1:B:253:GLN:O	2.21	0.41
1:C:57:MET:HE1	1:C:246:ILE:HG21	2.03	0.41
1:C:39:VAL:HG22	1:C:117:ILE:HD12	2.03	0.41
1:B:38:ILE:HG22	1:B:39:VAL:N	2.36	0.41
1:B:63:VAL:O	1:B:88:TYR:HA	2.21	0.40
1:C:121:ILE:HG23	2:C:503:NDP:H3D	2.03	0.40
1:D:131:ASP:N	1:D:131:ASP:OD2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:NDP:H2D	3:B:603:352:H19	2.03	0.40
1:D:239:GLU:H	1:D:239:GLU:CD	2.25	0.40
1:B:35:LYS:HD2	1:B:114:ASP:OD2	2.21	0.40
1:C:135:HIS:O	1:C:138:LYS:HB3	2.21	0.40
1:A:197:ILE:CG2	1:A:198:ARG:N	2.83	0.40
1:A:122:THR:HG22	1:A:143:ASN:OD1	2.21	0.40
1:B:78:CYS:C	1:B:80:GLU:H	2.24	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	257/275 (94%)	201 (78%)	44 (17%)	12 (5%)	3 17
1	B	253/275 (92%)	213 (84%)	34 (13%)	6 (2%)	7 35
1	C	254/275 (92%)	218 (86%)	32 (13%)	4 (2%)	12 48
1	D	259/275 (94%)	220 (85%)	32 (12%)	7 (3%)	6 32
All	All	1023/1100 (93%)	852 (83%)	142 (14%)	29 (3%)	6 30

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	225	LYS
1	B	65	ALA
1	B	220	THR
1	A	58	GLY
1	A	83	ALA
1	A	205	ARG
1	B	223	ALA

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Mol	Chain	Res	Type
1	C	205	ARG
1	D	45	GLY
1	D	65	ALA
1	D	227	VAL
1	A	84	ALA
1	B	80	GLU
1	A	65	ALA
1	A	86	ALA
1	A	115	MET
1	B	85	SER
1	C	219	ASP
1	D	96	MET
1	D	127	ASN
1	A	85	SER
1	C	65	ALA
1	D	69	GLU
1	A	219	ASP
1	B	265	THR
1	D	179	MET
1	A	230	ILE
1	C	230	ILE

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	216/232 (93%)	198 (92%)	18 (8%)	14 46
1	B	212/232 (91%)	202 (95%)	10 (5%)	32 72
1	C	213/232 (92%)	201 (94%)	12 (6%)	26 65
1	D	218/232 (94%)	204 (94%)	14 (6%)	22 59
All	All	859/928 (93%)	805 (94%)	54 (6%)	22 60

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	97	THR
1	A	100	GLU
1	A	101	GLN
1	A	118	LEU
1	A	119	ASN
1	A	134	HIS
1	A	141	GLU
1	A	170	SER
1	A	197	ILE
1	A	221	GLU
1	A	224	MET
1	A	239	GLU
1	A	247	LYS
1	A	266	LEU
1	A	270	ASN
1	A	272	SER
1	A	282	THR
1	B	36	LYS
1	B	108	LYS
1	B	123	ASN
1	B	150	LEU
1	B	197	ILE
1	B	222	THR
1	B	225	LYS
1	B	262	LEU
1	B	270	ASN
1	B	274	LYS
1	C	33	GLN
1	C	36	LYS
1	C	37	VAL
1	C	46	ILE
1	C	70	THR
1	C	73	LYS
1	C	160	GLN
1	C	205	ARG
1	C	207	ASN
1	C	243	LEU
1	C	272	SER
1	C	280	TYR
1	D	36	LYS
1	D	69	GLU
1	D	70	THR

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Mol	Chain	Res	Type
1	D	79	LEU
1	D	110	MET
1	D	127	ASN
1	D	141	GLU
1	D	150	LEU
1	D	170	SER
1	D	224	MET
1	D	243	LEU
1	D	252	ARG
1	D	270	ASN
1	D	285	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	105	GLN
1	A	120	HIS
1	A	127	ASN
1	A	162	ASN
1	A	253	GLN
1	A	270	ASN
1	B	53	HIS
1	B	101	GLN
1	B	105	GLN
1	B	120	HIS
1	B	134	HIS
1	B	135	HIS
1	B	270	ASN
1	C	105	GLN
1	C	162	ASN
1	C	207	ASN
1	C	253	GLN
1	D	33	GLN
1	D	53	HIS
1	D	72	GLN
1	D	120	HIS
1	D	123	ASN
1	D	127	ASN
1	D	130	HIS
1	D	270	ASN
1	D	285	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

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	NDP	A	501	-	42,52,52	1.47	6 (14%)	55,80,80	2.12	13 (23%)
3	352	A	601	-	21,22,22	2.30	8 (38%)	20,34,34	1.86	6 (30%)
2	NDP	B	502	-	42,52,52	1.56	7 (16%)	55,80,80	2.43	15 (27%)
3	352	B	603	-	21,22,22	1.96	7 (33%)	20,34,34	2.53	8 (40%)
2	NDP	C	503	-	42,52,52	1.25	5 (11%)	55,80,80	2.50	20 (36%)
3	352	C	602	-	21,22,22	1.83	5 (23%)	20,34,34	2.46	4 (20%)
2	NDP	D	504	-	42,52,52	1.53	7 (16%)	55,80,80	2.07	11 (20%)
3	352	D	604	-	21,22,22	2.12	7 (33%)	20,34,34	2.55	7 (35%)

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	NDP	A	501	-	-	0/30/77/77	0/5/5/5
3	352	A	601	-	-	0/8/32/32	0/2/2/2
2	NDP	B	502	-	-	0/30/77/77	0/5/5/5
3	352	B	603	-	-	0/8/32/32	0/2/2/2
2	NDP	C	503	-	1/1/14/17	0/30/77/77	0/5/5/5
3	352	C	602	-	-	0/8/32/32	0/2/2/2
2	NDP	D	504	-	-	0/30/77/77	0/5/5/5
3	352	D	604	-	-	0/8/32/32	0/2/2/2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	504	NDP	C4N-C5N	-4.26	1.39	1.49
2	B	502	NDP	C4N-C5N	-4.12	1.40	1.49
2	A	501	NDP	C4N-C5N	-4.09	1.40	1.49
2	C	503	NDP	C4N-C5N	-3.90	1.40	1.49
2	D	504	NDP	O4D-C4D	-2.28	1.39	1.45
2	D	504	NDP	O4B-C4B	-2.16	1.40	1.45
3	B	603	352	C4-C5	2.03	1.41	1.37
3	C	602	352	C4-C5	2.03	1.41	1.37
3	D	604	352	C11-N15	2.06	1.34	1.31
3	D	604	352	C7-C8	2.07	1.42	1.39
2	A	501	NDP	P2B-O1X	2.07	1.58	1.51
3	B	603	352	C13-C14	2.08	1.56	1.53
3	A	601	352	C10-N9	2.09	1.50	1.47
3	B	603	352	C7-C8	2.10	1.42	1.39
2	B	502	NDP	C2D-C1D	2.10	1.60	1.53
3	B	603	352	C3-C8	2.17	1.42	1.39
2	D	504	NDP	C2A-N1A	2.23	1.38	1.33
2	C	503	NDP	C2A-N1A	2.25	1.38	1.33
3	B	603	352	C6-C5	2.25	1.41	1.37
3	C	602	352	C6-C5	2.39	1.41	1.37
2	A	501	NDP	C2A-N3A	2.41	1.36	1.32
3	C	602	352	C7-C8	2.46	1.43	1.39
3	A	601	352	C7-C8	2.54	1.43	1.39
3	A	601	352	C7-C6	2.55	1.43	1.38
2	A	501	NDP	C2N-C3N	2.63	1.41	1.34
2	B	502	NDP	C4A-N3A	2.65	1.39	1.35
2	C	503	NDP	C2N-C3N	2.71	1.41	1.34
3	D	604	352	C6-C5	2.79	1.42	1.37
2	C	503	NDP	C2A-N3A	2.98	1.37	1.32
3	D	604	352	C3-C8	3.00	1.44	1.39
2	B	502	NDP	C2A-N3A	3.07	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	352	C11-N15	3.12	1.36	1.31
2	C	503	NDP	C6N-C5N	3.19	1.39	1.33
2	B	502	NDP	C2A-N1A	3.24	1.40	1.33
3	A	601	352	C13-C14	3.27	1.57	1.53
3	B	603	352	C11-N15	3.29	1.36	1.31
2	D	504	NDP	C2N-C3N	3.29	1.42	1.34
3	C	602	352	C11-N15	3.35	1.36	1.31
3	A	601	352	C6-C5	3.43	1.43	1.37
3	A	601	352	C11-S12	3.45	1.79	1.75
3	D	604	352	C7-C6	3.47	1.45	1.38
2	A	501	NDP	C6N-C5N	3.51	1.40	1.33
2	D	504	NDP	C2A-N3A	3.55	1.38	1.32
2	A	501	NDP	C2A-N1A	3.57	1.40	1.33
2	B	502	NDP	C2N-C3N	3.73	1.43	1.34
2	B	502	NDP	C6N-C5N	3.76	1.40	1.33
3	D	604	352	C11-N9	3.94	1.40	1.34
2	D	504	NDP	C6N-C5N	4.11	1.41	1.33
3	C	602	352	C11-N9	4.46	1.41	1.34
3	D	604	352	C13-C14	4.95	1.59	1.53
3	B	603	352	C11-N9	5.22	1.42	1.34
3	A	601	352	C11-N9	5.84	1.43	1.34

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	NDP	N3A-C2A-N1A	-11.28	120.26	128.89
2	B	502	NDP	N3A-C2A-N1A	-11.20	120.32	128.89
2	D	504	NDP	N3A-C2A-N1A	-9.93	121.29	128.89
2	C	503	NDP	N3A-C2A-N1A	-9.51	121.62	128.89
3	C	602	352	C21-C1-C2	-7.56	97.77	110.39
3	D	604	352	C19-C10-N9	-7.23	98.71	109.03
3	B	603	352	N9-C11-N15	-5.95	118.64	124.25
2	B	502	NDP	C4B-O4B-C1B	-5.66	103.49	109.72
3	D	604	352	N9-C11-N15	-5.08	119.46	124.25
3	B	603	352	C19-C10-N9	-4.36	102.81	109.03
2	C	503	NDP	C4N-C5N-C6N	-4.32	115.46	122.58
2	B	502	NDP	O2D-C2D-C3D	-4.10	98.51	111.83
3	D	604	352	C21-C1-C2	-4.02	103.68	110.39
2	C	503	NDP	C4D-O4D-C1D	-3.99	100.74	109.52
2	C	503	NDP	C2D-C3D-C4D	-3.81	94.79	102.61
3	A	601	352	C19-C10-N9	-3.77	103.65	109.03
2	D	504	NDP	C4N-C5N-C6N	-3.71	116.47	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	NDP	C1B-N9A-C4A	-3.53	121.62	126.94
3	A	601	352	C21-C1-C2	-3.46	104.61	110.39
3	B	603	352	C19-C10-C8	-3.43	105.35	112.16
2	C	503	NDP	O4B-C1B-C2B	-3.37	100.50	106.60
2	B	502	NDP	O3B-C3B-C4B	-3.29	101.18	111.05
2	C	503	NDP	C2D-C1D-N1N	-3.27	104.51	113.34
2	A	501	NDP	O4B-C1B-C2B	-3.19	100.82	106.60
2	B	502	NDP	C4N-C5N-C6N	-3.13	117.42	122.58
2	A	501	NDP	C4N-C5N-C6N	-3.10	117.46	122.58
2	B	502	NDP	O4B-C1B-C2B	-2.94	101.29	106.60
2	D	504	NDP	C3N-C2N-N1N	-2.93	118.94	123.14
2	D	504	NDP	O4B-C1B-C2B	-2.83	101.49	106.60
2	B	502	NDP	C3N-C2N-N1N	-2.80	119.13	123.14
3	B	603	352	C21-C1-C2	-2.80	105.71	110.39
2	A	501	NDP	C4A-C5A-N7A	-2.73	106.97	109.48
2	C	503	NDP	C4A-C5A-N7A	-2.63	107.06	109.48
3	B	603	352	O20-C1-C2	-2.49	100.30	107.38
2	C	503	NDP	C1D-N1N-C6N	-2.45	115.33	120.81
3	C	602	352	C19-C10-N9	-2.44	105.55	109.03
2	D	504	NDP	O3B-C3B-C4B	-2.42	103.78	111.05
2	A	501	NDP	O4D-C1D-C2D	-2.41	101.00	106.58
3	B	603	352	C7-C8-C10	-2.33	116.63	120.81
2	B	502	NDP	C4A-C5A-N7A	-2.30	107.36	109.48
2	C	503	NDP	C3N-C2N-N1N	-2.26	119.89	123.14
3	A	601	352	F18-C5-C4	-2.21	114.83	118.52
3	D	604	352	O20-C1-C2	-2.20	101.14	107.38
2	C	503	NDP	O3D-C3D-C2D	-2.20	104.69	111.83
3	A	601	352	O20-C1-C21	-2.11	101.39	107.38
2	A	501	NDP	C1B-N9A-C4A	-2.03	123.88	126.94
2	C	503	NDP	O5D-C5D-C4D	-2.00	101.74	109.12
2	D	504	NDP	C1D-N1N-C2N	2.01	124.41	120.91
2	A	501	NDP	O2B-C2B-C1B	2.09	118.16	110.02
2	A	501	NDP	O4D-C1D-N1N	2.11	112.52	108.07
3	C	602	352	C8-C10-N9	2.13	115.35	111.41
3	D	604	352	C4-C3-C8	2.15	123.42	121.20
2	B	502	NDP	O4B-C4B-C5B	2.23	117.31	109.32
2	A	501	NDP	O3B-C3B-C2B	2.23	117.61	111.16
3	D	604	352	C8-C10-N9	2.27	115.61	111.41
2	B	502	NDP	O4D-C1D-N1N	2.30	112.94	108.07
3	A	601	352	C8-C10-N9	2.36	115.77	111.41
2	C	503	NDP	C1D-N1N-C2N	2.49	125.24	120.91
2	B	502	NDP	O4D-C4D-C3D	2.53	110.25	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	503	NDP	O3B-C3B-C2B	2.59	118.65	111.16
2	D	504	NDP	O3-PN-O5D	2.61	109.85	102.94
2	A	501	NDP	O3B-C3B-C4B	2.71	119.17	111.05
2	B	502	NDP	O3-PA-O5B	2.74	110.20	102.94
2	D	504	NDP	C5N-C4N-C3N	2.80	120.23	112.52
2	C	503	NDP	C3B-C2B-C1B	2.81	108.17	102.73
2	A	501	NDP	C5N-C4N-C3N	2.87	120.42	112.52
2	C	503	NDP	O4D-C1D-N1N	2.89	114.17	108.07
2	D	504	NDP	O3D-C3D-C4D	3.00	120.04	111.05
3	D	604	352	O20-C1-C21	3.03	116.00	107.38
2	B	502	NDP	C5N-C4N-C3N	3.11	121.08	112.52
2	C	503	NDP	O3D-C3D-C4D	3.24	120.76	111.05
2	C	503	NDP	C5N-C4N-C3N	3.28	121.57	112.52
2	A	501	NDP	O3-PA-O5B	3.34	111.80	102.94
3	A	601	352	F18-C5-C6	3.70	124.70	118.52
3	B	603	352	O20-C1-C21	3.78	118.12	107.38
2	A	501	NDP	O2D-C2D-C1D	3.85	123.40	109.94
2	B	502	NDP	O2D-C2D-C1D	4.27	124.84	109.94
2	D	504	NDP	C4B-O4B-C1B	4.43	114.59	109.72
3	B	603	352	C8-C10-N9	4.49	119.72	111.41
2	D	504	NDP	O2D-C2D-C1D	4.53	125.77	109.94
2	C	503	NDP	C4B-O4B-C1B	4.71	114.90	109.72
2	C	503	NDP	O4D-C4D-C5D	4.99	127.16	109.32
2	C	503	NDP	O2D-C2D-C1D	5.01	127.45	109.94
3	C	602	352	O20-C1-C21	6.27	125.21	107.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	503	NDP	C4D

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NDP	5	0
2	B	502	NDP	5	0
3	B	603	352	3	0
2	C	503	NDP	3	0
2	D	504	NDP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	604	352	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	259/275 (94%)	-0.11	5 (1%) 70 41	23, 54, 80, 98	0
1	B	255/275 (92%)	-0.37	0 100 100	21, 43, 65, 80	0
1	C	256/275 (93%)	-0.52	0 100 100	13, 35, 57, 73	0
1	D	261/275 (94%)	-0.41	2 (0%) 87 67	16, 36, 65, 93	0
All	All	1031/1100 (93%)	-0.35	7 (0%) 89 70	13, 41, 71, 98	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	VAL	7.8
1	D	230	ILE	6.0
1	A	232	HIS	5.5
1	D	229	GLY	3.2
1	A	32	LEU	2.9
1	A	85	SER	2.2
1	A	54	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
3	352	B	603	21/21	0.95	0.22	0.73	32,35,39,40	0
3	352	C	602	21/21	0.96	0.18	0.13	24,27,29,29	0
3	352	A	601	21/21	0.94	0.17	-0.36	34,38,41,41	0
2	NDP	D	504	48/48	0.96	0.14	-0.45	21,28,32,34	0
2	NDP	C	503	48/48	0.96	0.15	-0.63	25,32,35,36	0
3	352	D	604	21/21	0.96	0.15	-0.68	22,26,32,34	0
2	NDP	B	502	48/48	0.96	0.14	-1.10	30,36,39,40	0
2	NDP	A	501	48/48	0.96	0.14	-1.32	30,33,36,37	0

6.5 Other polymers

There are no such residues in this entry.