



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:33 am GMT

PDB ID : 1EBU
Title : HOMOSERINE DEHYDROGENASE COMPLEX WITH NAD ANALOGUE
AND L-HOMOSERINE
Authors : DeLaBarre, B.; Thompson, P.R.; Wright, G.D.; Berghuis, A.M.
Deposited on : 2000-01-24
Resolution : 2.60 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

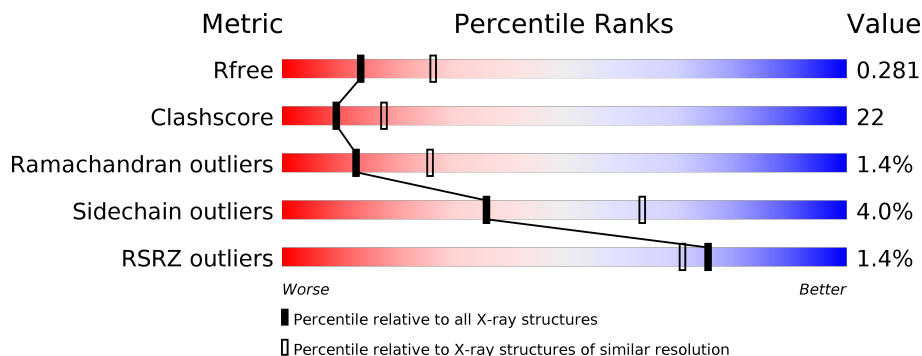
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 $\leq 5\%$. 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	358	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>34%</div> <div>.</div> </div> </div>
1	B	358	<div> <div></div> <div> <div>65%</div> <div>30%</div> <div>.</div> </div> </div>
1	C	358	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>34%</div> <div>.</div> </div> </div>
1	D	358	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>.</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	A	901	-	-	-	X
3	NDA	D	1300	-	-	-	X
4	HSE	D	1301	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11246 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.

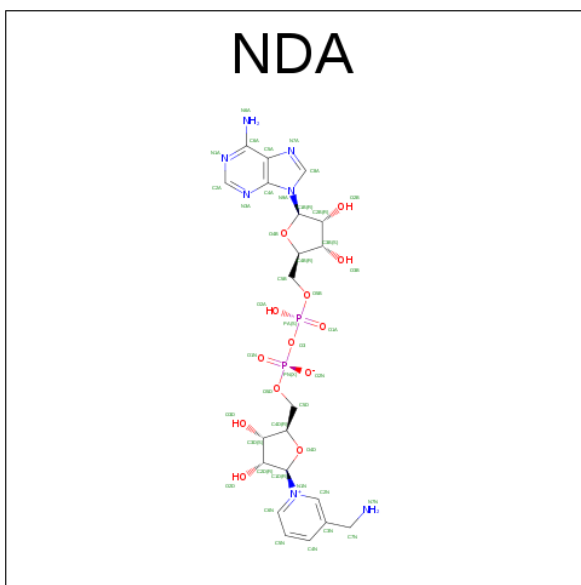
- Molecule 1 is a protein called HOMOSERINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2710	1737	443	529	1			
1	B	358	Total	C	N	O	S	0	0	0
			2710	1737	443	529	1			
1	C	358	Total	C	N	O	S	0	0	0
			2710	1737	443	529	1			
1	D	358	Total	C	N	O	S	0	0	0
			2710	1737	443	529	1			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

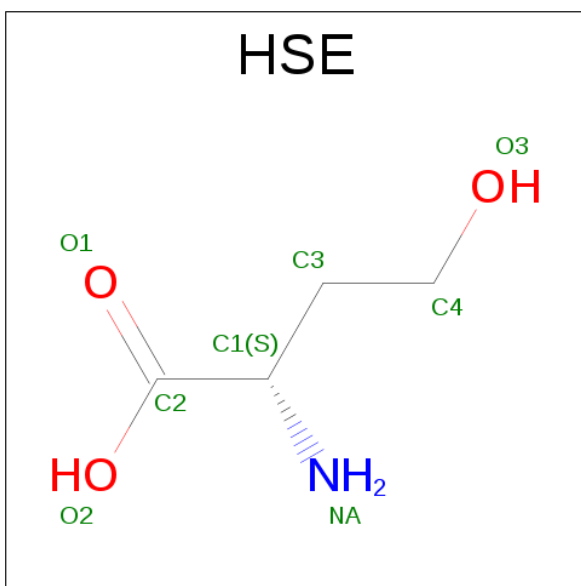
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

- Molecule 3 is 3-AMINOMETHYL-PYRIDINIUM-ADENINE-DINUCLEOTIDE (three-letter code: NDA) (formula: C₂₁H₂₉N₇O₁₃P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total 43	C 21	N 7	O 13	P 2	0	0

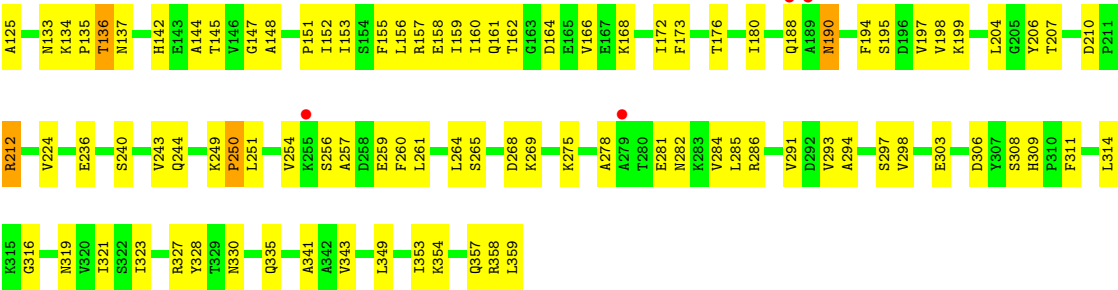
- Molecule 4 is L-HOMOSERINE (three-letter code: HSE) (formula: $\text{C}_4\text{H}_9\text{NO}_3$).



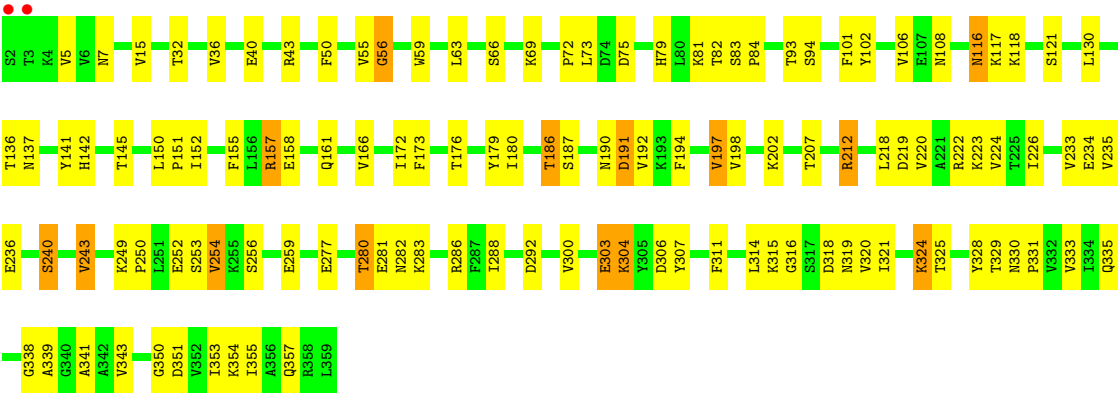
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total 71	O 71	0	0
5	B	100	Total 100	O 100	0	0
5	C	75	Total 75	O 75	0	0
5	D	105	Total 105	O 105	0	0



● Molecule 1: HOMOSERINE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.78Å 104.09Å 120.64Å 90.00° 91.93° 90.00°	Depositor
Resolution (Å)	39.40 – 2.60 39.40 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.40-2.60) 99.2 (39.40-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 2.61Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.215 , 0.283 0.217 , 0.281	Depositor DCC
R_{free} test set	4028 reflections (9.07%)	DCC
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11246	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: NDA, NA, HSE

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	0.43	0/2757	0.70	1/3741 (0.0%)
1	B	0.43	0/2757	0.72	5/3741 (0.1%)
1	C	0.37	0/2757	0.66	1/3741 (0.0%)
1	D	0.39	0/2757	0.68	2/3741 (0.1%)
All	All	0.41	0/11028	0.69	9/14964 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	ALA	N-CA-C	-8.41	88.30	111.00
1	B	286	ARG	NE-CZ-NH1	-7.83	116.38	120.30
1	D	254	VAL	N-CA-C	-6.27	94.08	111.00
1	B	280	THR	N-CA-C	-5.99	94.82	111.00
1	B	279	ALA	N-CA-C	-5.46	96.27	111.00
1	B	281	GLU	N-CA-C	-5.29	96.71	111.00
1	A	134	LYS	N-CA-C	-5.22	96.89	111.00
1	D	292	ASP	N-CA-C	-5.14	97.13	111.00
1	C	330	ASN	N-CA-C	-5.07	97.30	111.00

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	2710	0	2782	141	0
1	B	2710	0	2782	123	0
1	C	2710	0	2782	114	0
1	D	2710	0	2782	109	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	D	43	0	28	3	0
4	D	8	0	8	1	0
5	A	71	0	0	4	0
5	B	100	0	0	4	0
5	C	75	0	0	7	0
5	D	105	0	0	5	0
All	All	11246	0	11164	476	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 22.

All (476) 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:D:320:VAL:HG12	1:D:335:GLN:HB2	1.26	1.15
1:B:117:LYS:HG2	1:B:145:THR:HG23	1.41	1.02
1:C:28:LYS:HD2	1:C:28:LYS:H	1.28	0.99
1:D:79:HIS:O	1:D:82:THR:HG22	1.64	0.98
1:D:5:VAL:HG22	1:D:32:THR:HB	1.47	0.94
1:C:106:VAL:HG12	1:C:137:ASN:HB2	1.47	0.93
1:B:172:ILE:O	1:B:319:ASN:HB2	1.70	0.92
1:D:172:ILE:O	1:D:319:ASN:HB2	1.71	0.91
1:B:152:ILE:HD12	1:B:321:ILE:HG21	1.54	0.90
1:B:278:ALA:O	5:B:644:HOH:O	1.88	0.90
1:A:37:LEU:HD23	1:A:46:ILE:HB	1.54	0.90
1:B:202:LYS:HA	1:B:207:THR:HG22	1.53	0.89
1:D:339:ALA:HA	3:D:1300:NDA:H4N	1.55	0.89
1:C:58:ASP:HB2	5:C:632:HOH:O	1.74	0.87
1:A:176:THR:HG23	1:A:207:THR:HG22	1.59	0.85
1:C:309:HIS:HD2	1:C:311:PHE:H	1.25	0.84
1:D:55:VAL:HG11	1:D:59:TRP:HA	1.58	0.84
1:D:117:LYS:HG2	1:D:145:THR:HG23	1.58	0.83
1:A:27:MET:HE2	1:A:353:ILE:HD11	1.62	0.82
1:A:28:LYS:HD2	1:A:28:LYS:H	1.45	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:VAL:HG12	1:B:335:GLN:HB2	1.62	0.81
1:B:319:ASN:HD21	1:B:338:GLY:HA3	1.45	0.80
1:B:212:ARG:HG3	1:B:212:ARG:HH11	1.49	0.78
1:A:156:LEU:O	1:A:160:ILE:HG12	1.84	0.77
1:C:249:LYS:HB2	1:C:250:PRO:HD3	1.66	0.77
1:B:116:ASN:HD21	1:B:118:LYS:HG2	1.50	0.77
1:C:34:ASN:CG	1:C:52:PRO:HG3	2.06	0.77
1:D:286:ARG:HB3	1:D:286:ARG:NH1	2.00	0.76
1:B:353:ILE:O	1:B:357:GLN:HG3	1.85	0.76
1:A:27:MET:CE	1:A:353:ILE:HD11	2.15	0.76
1:B:145:THR:HG21	1:B:226:ILE:HD13	1.68	0.75
1:B:202:LYS:HA	1:B:207:THR:CG2	2.17	0.75
1:D:320:VAL:HG12	1:D:335:GLN:CB	2.14	0.75
1:D:43:ARG:HB2	1:D:43:ARG:NH1	2.02	0.74
1:B:2:SER:HB2	1:B:30:THR:O	1.88	0.73
1:C:28:LYS:HD2	1:C:28:LYS:N	2.00	0.73
1:D:212:ARG:NH2	1:D:254:VAL:O	2.21	0.73
1:B:190:ASN:HD22	1:B:192:VAL:HG22	1.52	0.73
1:A:152:ILE:HG21	1:A:321:ILE:HD12	1.71	0.73
1:B:280:THR:O	1:B:281:GLU:HB2	1.88	0.73
1:D:319:ASN:ND2	1:D:338:GLY:HA3	2.04	0.72
1:B:212:ARG:HD3	1:B:260:PHE:CD1	2.24	0.72
1:A:106:VAL:HG12	1:A:137:ASN:HB2	1.72	0.72
1:A:28:LYS:HD2	1:A:28:LYS:N	2.04	0.72
1:C:135:PRO:O	1:C:136:THR:HG23	1.90	0.71
1:D:212:ARG:HH21	1:D:254:VAL:HG22	1.54	0.71
1:D:212:ARG:HH21	1:D:254:VAL:CG2	2.04	0.70
1:A:195:SER:OG	1:A:265:SER:HA	1.91	0.70
1:C:190:ASN:C	1:C:190:ASN:HD22	1.93	0.70
1:A:147:GLY:HA3	1:A:152:ILE:HD12	1.74	0.70
1:B:146:VAL:HB	1:B:153:ILE:HD11	1.74	0.70
1:C:256:SER:OG	1:C:259:GLU:HG3	1.92	0.69
1:A:159:ILE:HG23	1:A:164:ASP:HB3	1.74	0.69
1:A:254:VAL:CG2	1:A:259:GLU:HB2	2.22	0.69
1:B:249:LYS:HB2	1:B:250:PRO:HD3	1.75	0.69
1:C:152:ILE:HD13	1:C:321:ILE:CD1	2.23	0.69
1:C:37:LEU:CD2	1:C:46:ILE:HB	2.23	0.68
1:B:210:ASP:OD1	1:B:212:ARG:HG3	1.93	0.68
1:A:251:LEU:N	1:A:251:LEU:HD12	2.09	0.68
1:C:27:MET:HE2	1:C:353:ILE:HD11	1.76	0.68
1:B:304:LYS:HB3	1:B:304:LYS:NZ	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ASN:HB2	1:B:307:TYR:CD1	2.29	0.68
1:D:152:ILE:HD12	1:D:321:ILE:HG21	1.75	0.68
1:D:288:ILE:HD11	1:D:303:GLU:OE1	1.94	0.68
1:C:27:MET:HE3	1:C:349:LEU:HD21	1.75	0.67
1:C:198:VAL:HG21	1:C:264:LEU:CD2	2.25	0.67
1:C:195:SER:OG	1:C:265:SER:HA	1.94	0.67
1:D:69:LYS:HG3	5:D:437:HOH:O	1.94	0.67
1:A:34:ASN:OD1	1:A:52:PRO:HG3	1.95	0.66
1:D:55:VAL:CG1	1:D:59:TRP:HA	2.26	0.66
1:B:278:ALA:O	1:B:279:ALA:HB2	1.96	0.66
1:D:116:ASN:HD22	1:D:117:LYS:N	1.93	0.66
1:B:36:VAL:HG11	1:B:50:PHE:CD2	2.31	0.65
1:A:108:ASN:N	1:A:108:ASN:HD22	1.92	0.65
1:A:152:ILE:HD13	1:A:321:ILE:CD1	2.27	0.65
1:A:37:LEU:CD2	1:A:46:ILE:HB	2.26	0.65
1:D:190:ASN:OD1	1:D:192:VAL:HG13	1.97	0.65
1:A:81:LYS:HB3	1:A:81:LYS:NZ	2.12	0.65
1:D:141:TYR:HB3	1:D:351:ASP:OD2	1.97	0.64
1:A:195:SER:O	1:A:198:VAL:HG22	1.97	0.64
1:B:324:LYS:NZ	1:B:329:THR:HA	2.12	0.64
1:A:254:VAL:HG21	1:A:260:PHE:N	2.13	0.64
1:A:198:VAL:HG21	1:A:264:LEU:CD2	2.28	0.64
1:C:354:LYS:HE2	1:D:158:GLU:OE2	1.97	0.64
1:A:254:VAL:HG22	1:A:259:GLU:HB2	1.79	0.64
1:B:30:THR:HG23	1:B:31:ILE:H	1.62	0.64
1:A:224:VAL:HG21	1:A:289:GLY:HA3	1.80	0.64
1:A:30:THR:HG23	1:A:31:ILE:H	1.62	0.64
1:A:159:ILE:CG2	1:A:164:ASP:HB3	2.28	0.63
1:A:94:SER:O	1:A:118:LYS:HE3	1.97	0.63
1:C:212:ARG:HD2	1:C:260:PHE:CG	2.34	0.63
1:D:15:VAL:HG12	1:D:341:ALA:HB2	1.80	0.63
1:D:319:ASN:HD21	1:D:338:GLY:HA3	1.61	0.63
1:C:106:VAL:CG1	1:C:137:ASN:HB2	2.26	0.63
1:B:58:ASP:HA	5:B:543:HOH:O	1.98	0.63
1:D:180:ILE:HG23	1:D:197:VAL:HG22	1.80	0.62
1:A:126:THR:O	1:A:130:LEU:HG	2.00	0.62
1:B:190:ASN:ND2	1:B:192:VAL:HG13	2.13	0.62
1:B:286:ARG:O	1:B:288:ILE:HG23	1.99	0.62
1:B:55:VAL:HG11	1:B:59:TRP:HB3	1.81	0.62
1:A:142:HIS:HE1	1:A:157:ARG:HH21	1.47	0.62
1:B:212:ARG:NH1	1:B:212:ARG:HG3	2.11	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:LYS:HA	1:D:207:THR:HG22	1.81	0.62
1:B:55:VAL:HG11	1:B:59:TRP:CB	2.29	0.62
1:C:156:LEU:O	1:C:160:ILE:HG12	1.98	0.62
1:A:184:PHE:CZ	1:A:275:LYS:HD3	2.35	0.62
1:B:212:ARG:HD3	1:B:260:PHE:CG	2.34	0.62
1:C:284:VAL:HG22	1:C:286:ARG:HH12	1.65	0.62
1:B:320:VAL:HG12	1:B:335:GLN:CB	2.30	0.61
1:D:145:THR:HG21	1:D:226:ILE:HD13	1.82	0.61
1:D:145:THR:HG21	1:D:226:ILE:CD1	2.30	0.61
1:D:40:GLU:HG3	1:D:63:LEU:HD21	1.83	0.61
1:A:190:ASN:ND2	1:A:192:VAL:H	1.99	0.61
1:C:34:ASN:OD1	1:C:52:PRO:HG3	2.00	0.61
1:A:146:VAL:HG23	1:A:153:ILE:HD11	1.82	0.61
1:A:49:ASP:O	1:A:50:PHE:HB2	2.00	0.61
1:D:282:ASN:HA	1:D:307:TYR:CE1	2.36	0.61
1:C:172:ILE:HD12	1:C:314:LEU:HD11	1.83	0.60
1:C:27:MET:CE	1:C:353:ILE:HD11	2.31	0.60
1:C:37:LEU:HD23	1:C:46:ILE:HD12	1.82	0.60
1:C:30:THR:HG23	1:C:31:ILE:N	2.17	0.60
1:B:166:VAL:HA	1:B:325:THR:HG22	1.83	0.60
1:C:49:ASP:O	1:C:50:PHE:HB2	2.02	0.60
1:D:353:ILE:O	1:D:357:GLN:HG3	2.01	0.60
1:A:152:ILE:HG21	1:A:321:ILE:CD1	2.32	0.59
1:C:198:VAL:HG21	1:C:264:LEU:HD23	1.85	0.59
1:C:142:HIS:HE1	1:C:157:ARG:HH21	1.50	0.59
1:D:202:LYS:HA	1:D:207:THR:CG2	2.32	0.59
1:B:44:SER:O	1:B:68:THR:HB	2.02	0.59
1:A:107:GLU:C	1:A:108:ASN:HD22	2.06	0.59
1:A:152:ILE:HD13	1:A:321:ILE:HD12	1.83	0.59
1:A:254:VAL:HG21	1:A:260:PHE:H	1.67	0.59
1:B:286:ARG:CZ	1:B:286:ARG:HB3	2.32	0.59
1:A:288:ILE:HD13	1:A:305:TYR:OH	2.02	0.58
1:A:106:VAL:CG1	1:A:137:ASN:HB2	2.33	0.58
1:A:159:ILE:HG23	1:A:164:ASP:CB	2.33	0.58
1:C:37:LEU:HD22	1:C:46:ILE:HB	1.86	0.58
1:B:196:ASP:O	1:B:200:VAL:HG23	2.03	0.58
1:D:55:VAL:HG11	1:D:59:TRP:CA	2.31	0.58
1:C:251:LEU:O	1:C:254:VAL:HG22	2.03	0.58
1:B:190:ASN:HD21	1:B:192:VAL:HG13	1.67	0.58
1:C:194:PHE:O	1:C:197:VAL:HG22	2.02	0.58
1:D:218:LEU:O	1:D:222:ARG:HG3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:THR:HG23	1:A:31:ILE:N	2.19	0.57
1:A:152:ILE:CG2	1:A:321:ILE:HD12	2.33	0.57
1:C:176:THR:HG23	1:C:207:THR:HG22	1.87	0.57
1:B:145:THR:HG21	1:B:226:ILE:CD1	2.34	0.57
1:A:176:THR:CG2	1:A:207:THR:HG22	2.34	0.57
1:A:327:ARG:NH1	1:B:346:ALA:HB2	2.20	0.57
1:C:358:ARG:O	1:C:359:LEU:HB2	2.05	0.57
1:A:265:SER:HB2	5:A:667:HOH:O	2.05	0.56
1:B:243:VAL:HB	1:B:300:VAL:CG2	2.35	0.56
1:D:288:ILE:C	1:D:288:ILE:HD12	2.25	0.56
1:D:50:PHE:CD1	1:D:84:PRO:HD3	2.41	0.56
1:A:291:VAL:HG22	1:A:298:VAL:HG22	1.88	0.56
1:B:77:ILE:O	1:B:81:LYS:HG2	2.06	0.56
1:B:278:ALA:HB1	1:B:283:LYS:O	2.06	0.56
1:A:194:PHE:O	1:A:197:VAL:HG22	2.06	0.55
1:C:343:VAL:HG13	1:D:328:TYR:OH	2.06	0.55
1:C:99:ALA:HB1	1:C:119:ALA:HB2	1.88	0.55
1:B:141:TYR:HB3	1:B:351:ASP:OD2	2.06	0.55
1:C:50:PHE:CE2	1:C:83:SER:HB2	2.42	0.55
1:A:249:LYS:HB2	1:A:250:PRO:HD3	1.89	0.54
1:B:55:VAL:CG1	1:B:59:TRP:HA	2.37	0.54
1:A:226:ILE:O	1:A:230:ILE:HG13	2.07	0.54
1:B:152:ILE:CD1	1:B:321:ILE:HG21	2.32	0.54
1:D:190:ASN:OD1	1:D:192:VAL:N	2.40	0.54
1:A:73:LEU:HD12	1:A:101:PHE:CE1	2.42	0.54
1:C:275:LYS:O	1:C:278:ALA:HB3	2.07	0.54
1:D:286:ARG:HB3	1:D:286:ARG:HH11	1.68	0.54
1:A:81:LYS:HB3	1:A:81:LYS:HZ3	1.70	0.54
1:B:319:ASN:HD21	1:B:338:GLY:CA	2.18	0.54
1:D:277:GLU:O	1:D:280:THR:N	2.35	0.54
1:A:123:ASP:OD2	1:A:126:THR:N	2.36	0.54
1:D:116:ASN:HD21	1:D:118:LYS:HG2	1.73	0.54
3:D:1300:NDA:HC72	4:D:1301:HSE:H1	1.90	0.54
1:A:103:THR:O	1:A:107:GLU:HG2	2.08	0.54
1:A:265:SER:HA	1:A:268:ASP:OD2	2.08	0.54
1:C:152:ILE:HD13	1:C:321:ILE:HD12	1.90	0.54
1:D:249:LYS:HB2	1:D:250:PRO:HD3	1.90	0.54
1:B:309:HIS:CE1	1:B:310:PRO:HD2	2.43	0.54
1:C:158:GLU:O	1:C:162:THR:HG23	2.08	0.54
1:B:91:ASP:O	1:B:115:PRO:HD2	2.08	0.53
1:C:89:LEU:HD22	1:C:105:PHE:CE2	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:THR:HG23	1:C:31:ILE:H	1.73	0.53
1:B:126:THR:O	1:B:130:LEU:HG	2.08	0.53
1:D:283:LYS:HG2	1:D:306:ASP:HA	1.90	0.53
1:A:212:ARG:HD2	1:A:260:PHE:CG	2.44	0.53
1:D:256:SER:HB3	1:D:259:GLU:HB2	1.90	0.53
1:A:91:ASP:O	1:A:115:PRO:HD2	2.08	0.53
1:A:155:PHE:CD1	1:B:151:PRO:HG3	2.43	0.53
1:B:309:HIS:CD2	1:B:311:PHE:H	2.26	0.53
1:B:209:PRO:O	1:B:211:PRO:HD3	2.09	0.53
1:B:30:THR:HG23	1:B:31:ILE:N	2.23	0.53
1:D:320:VAL:CG1	1:D:335:GLN:HB2	2.18	0.53
1:B:311:PHE:HA	1:B:314:LEU:CD1	2.38	0.53
1:B:280:THR:O	1:B:280:THR:HG23	2.08	0.53
1:B:324:LYS:HZ3	1:B:329:THR:HA	1.73	0.53
1:D:116:ASN:ND2	1:D:118:LYS:H	2.06	0.53
1:B:249:LYS:O	1:B:252:GLU:HG3	2.09	0.53
1:A:233:VAL:O	1:A:235:VAL:HG23	2.08	0.53
1:C:135:PRO:O	1:C:136:THR:CG2	2.57	0.53
1:A:73:LEU:HD12	1:A:101:PHE:CD1	2.44	0.52
1:C:152:ILE:HG21	1:C:321:ILE:HD12	1.92	0.52
1:A:190:ASN:ND2	1:A:192:VAL:N	2.58	0.52
1:A:198:VAL:HG21	1:A:264:LEU:HD23	1.92	0.52
1:A:187:SER:HA	1:A:307:TYR:CZ	2.44	0.52
1:A:267:TYR:N	1:A:267:TYR:CD1	2.77	0.52
1:A:218:LEU:O	1:A:222:ARG:HG3	2.09	0.52
1:A:224:VAL:CG2	1:A:289:GLY:HA3	2.39	0.52
1:B:277:GLU:O	1:B:280:THR:HG22	2.10	0.52
1:B:128:LYS:HZ1	1:B:234:GLU:CD	2.13	0.52
1:C:257:ALA:O	1:C:261:LEU:HB2	2.10	0.52
1:D:249:LYS:O	1:D:252:GLU:HG3	2.09	0.52
1:A:212:ARG:HD2	1:A:260:PHE:CD1	2.45	0.52
1:A:251:LEU:H	1:A:251:LEU:HD12	1.75	0.52
1:D:233:VAL:O	1:D:235:VAL:N	2.42	0.52
1:D:286:ARG:HH11	1:D:286:ARG:CB	2.23	0.52
1:D:286:ARG:HD2	1:D:311:PHE:HB3	1.91	0.52
1:D:43:ARG:HH11	1:D:43:ARG:HB2	1.71	0.52
1:A:195:SER:OG	1:A:265:SER:CA	2.58	0.51
1:A:273:GLN:O	1:A:277:GLU:HG3	2.10	0.51
1:C:166:VAL:O	1:C:293:VAL:HG21	2.10	0.51
1:C:152:ILE:HD13	1:C:321:ILE:HD11	1.91	0.51
1:C:15:VAL:HG12	1:C:341:ALA:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LYS:HD3	1:D:108:ASN:HB3	1.91	0.51
1:D:106:VAL:HG12	1:D:137:ASN:HB3	1.92	0.51
1:B:146:VAL:HB	1:B:153:ILE:CD1	2.39	0.51
1:C:99:ALA:HA	1:C:102:TYR:CE2	2.45	0.51
1:C:328:TYR:OH	1:D:343:VAL:HG13	2.11	0.51
1:A:134:LYS:HA	1:A:134:LYS:HE2	1.93	0.51
1:B:309:HIS:ND1	1:B:310:PRO:HD2	2.26	0.51
1:C:281:GLU:O	1:C:282:ASN:HB2	2.10	0.51
1:B:116:ASN:HD21	1:B:118:LYS:CG	2.22	0.51
1:C:224:VAL:CG1	1:C:298:VAL:HG13	2.40	0.51
1:C:251:LEU:HD12	1:C:251:LEU:N	2.26	0.51
1:C:284:VAL:CG2	1:C:286:ARG:HH12	2.24	0.51
1:D:142:HIS:HE1	1:D:157:ARG:HH21	1.58	0.51
1:B:281:GLU:CB	1:B:283:LYS:HE3	2.41	0.51
1:A:190:ASN:HD22	1:A:192:VAL:N	2.09	0.50
1:A:197:VAL:HG23	1:A:198:VAL:N	2.26	0.50
1:B:278:ALA:O	1:B:279:ALA:CB	2.56	0.50
1:C:243:VAL:HG13	1:C:243:VAL:O	2.11	0.50
1:C:72:PRO:HD2	1:C:75:ASP:OD2	2.11	0.50
1:D:7:ASN:HB3	1:D:36:VAL:HG21	1.94	0.50
1:A:209:PRO:O	1:A:211:PRO:HD3	2.11	0.50
1:A:251:LEU:N	1:A:251:LEU:CD1	2.74	0.50
1:D:324:LYS:HE2	1:D:329:THR:O	2.12	0.50
1:A:142:HIS:HE1	1:A:157:ARG:NH2	2.08	0.50
1:B:153:ILE:N	1:B:153:ILE:HD12	2.25	0.50
1:A:309:HIS:HD2	1:A:311:PHE:H	1.60	0.49
1:A:349:LEU:HD23	1:B:162:THR:HG22	1.94	0.49
1:B:269:LYS:HD3	5:B:755:HOH:O	2.12	0.49
1:A:190:ASN:HD22	1:A:192:VAL:H	1.57	0.49
1:D:350:GLY:O	1:D:354:LYS:HG3	2.13	0.49
1:A:167:GLU:O	1:A:293:VAL:HG22	2.13	0.49
1:B:186:THR:HG22	1:B:190:ASN:HB2	1.94	0.49
1:B:90:VAL:HG12	1:B:92:ASN:ND2	2.28	0.49
1:C:190:ASN:C	1:C:190:ASN:ND2	2.65	0.49
1:B:172:ILE:HG12	1:B:288:ILE:HG22	1.94	0.49
1:D:102:TYR:HB3	1:D:130:LEU:HD21	1.93	0.49
1:A:251:LEU:H	1:A:251:LEU:CD1	2.26	0.49
1:A:353:ILE:O	1:A:357:GLN:HG3	2.12	0.49
1:B:309:HIS:HD2	1:B:311:PHE:HB2	1.78	0.49
1:C:236:GLU:HB2	1:C:240:SER:CB	2.43	0.49
1:C:71:LEU:HG	5:C:565:HOH:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ILE:HD12	1:A:314:LEU:HD11	1.95	0.49
1:C:244:GLN:O	1:C:244:GLN:HG2	2.12	0.49
1:C:37:LEU:HD23	1:C:46:ILE:HB	1.93	0.49
1:D:173:PHE:HB3	1:D:223:LYS:CD	2.42	0.49
1:A:212:ARG:HG2	1:A:212:ARG:HH11	1.78	0.48
1:B:15:VAL:HG12	1:B:341:ALA:HB2	1.95	0.48
1:A:243:VAL:O	1:A:243:VAL:HG13	2.12	0.48
1:C:74:ASP:OD1	1:C:104:LYS:HE2	2.13	0.48
1:B:216:ASN:OD1	1:B:218:LEU:HB3	2.13	0.48
1:A:190:ASN:ND2	1:A:192:VAL:HB	2.29	0.48
1:B:207:THR:HG23	1:B:208:GLU:O	2.14	0.48
1:C:198:VAL:HG23	1:C:199:LYS:N	2.28	0.48
1:A:134:LYS:CA	1:A:134:LYS:HE2	2.43	0.48
1:D:116:ASN:C	1:D:116:ASN:HD22	2.16	0.48
1:A:28:LYS:H	1:A:28:LYS:CD	2.20	0.48
1:B:116:ASN:ND2	1:B:118:LYS:HG2	2.24	0.48
1:B:55:VAL:CG1	1:B:59:TRP:HB3	2.42	0.48
1:C:144:ALA:HA	1:C:148:ALA:O	2.14	0.48
1:D:351:ASP:O	1:D:355:ILE:HG13	2.14	0.48
1:B:157:ARG:HH11	1:B:157:ARG:HG3	1.78	0.48
1:D:102:TYR:O	1:D:106:VAL:HG23	2.14	0.48
1:C:160:ILE:HD11	1:C:166:VAL:HG23	1.96	0.48
1:C:284:VAL:HG22	1:C:286:ARG:NH1	2.29	0.48
1:C:168:LYS:HA	1:C:291:VAL:O	2.13	0.48
1:D:243:VAL:HA	1:D:300:VAL:HG22	1.95	0.48
1:A:99:ALA:HB1	1:A:119:ALA:HB2	1.96	0.47
1:B:286:ARG:HD3	1:B:311:PHE:HB3	1.95	0.47
1:B:296:LYS:HD2	1:B:296:LYS:N	2.29	0.47
1:B:304:LYS:HB3	1:B:304:LYS:HZ3	1.77	0.47
1:C:40:GLU:HB3	1:C:41:ALA:H	1.48	0.47
1:C:28:LYS:CD	1:C:28:LYS:H	2.12	0.47
1:D:72:PRO:HB2	1:D:75:ASP:OD2	2.14	0.47
1:A:248:PRO:HB2	1:A:251:LEU:HD13	1.96	0.47
1:B:2:SER:CB	1:B:30:THR:O	2.59	0.47
1:C:151:PRO:HD3	1:D:155:PHE:CE1	2.50	0.47
1:D:173:PHE:HB3	1:D:223:LYS:HD2	1.96	0.47
1:A:190:ASN:HD21	1:A:192:VAL:HB	1.79	0.47
1:A:335:GLN:HG2	1:B:333:VAL:HB	1.96	0.47
1:B:145:THR:CG2	1:B:226:ILE:CD1	2.93	0.47
1:C:155:PHE:O	1:C:159:ILE:HG12	2.14	0.47
1:B:134:LYS:HB2	1:B:137:ASN:CG	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:O	1:B:77:ILE:HG13	2.15	0.47
1:D:116:ASN:HD21	1:D:118:LYS:CG	2.28	0.47
1:A:333:VAL:HB	1:B:335:GLN:HG2	1.96	0.47
1:C:269:LYS:HE2	5:C:711:HOH:O	2.15	0.47
1:C:293:VAL:HG23	1:C:294:ALA:N	2.30	0.47
1:A:159:ILE:HA	1:A:159:ILE:HD13	1.75	0.47
1:C:133:ASN:ND2	5:C:463:HOH:O	2.48	0.47
1:D:277:GLU:O	1:D:280:THR:HB	2.15	0.47
1:A:329:THR:HA	5:A:745:HOH:O	2.16	0.46
1:B:291:VAL:HG22	1:B:298:VAL:HG22	1.96	0.46
1:D:176:THR:O	1:D:180:ILE:HG13	2.14	0.46
1:C:142:HIS:HB2	1:C:145:THR:CG2	2.45	0.46
1:C:102:TYR:O	1:C:106:VAL:HG23	2.16	0.46
1:C:212:ARG:HD2	1:C:260:PHE:CD1	2.51	0.46
1:C:27:MET:HE3	1:C:349:LEU:CD2	2.44	0.46
1:B:311:PHE:CE1	1:B:320:VAL:HG21	2.51	0.46
1:C:180:ILE:HD13	1:C:198:VAL:HG12	1.96	0.46
1:D:150:LEU:HA	1:D:151:PRO:HD3	1.80	0.46
1:B:123:ASP:OD2	1:B:125:ALA:HB3	2.15	0.46
1:C:135:PRO:O	1:C:136:THR:CB	2.63	0.46
1:C:309:HIS:CD2	1:C:311:PHE:H	2.16	0.46
1:A:50:PHE:CE2	1:A:83:SER:HB2	2.50	0.46
5:A:748:HOH:O	1:B:315:LYS:HG3	2.15	0.46
1:C:122:SER:OG	1:C:123:ASP:N	2.49	0.46
1:D:136:THR:O	1:D:136:THR:HG22	2.14	0.46
1:A:254:VAL:HG11	1:A:260:PHE:HB2	1.97	0.45
1:A:356:ALA:O	1:A:358:ARG:O	2.35	0.45
1:C:152:ILE:CG2	1:C:321:ILE:HD12	2.46	0.45
1:D:220:VAL:O	1:D:224:VAL:HG23	2.17	0.45
1:C:91:ASP:O	1:C:115:PRO:HD2	2.16	0.45
1:D:157:ARG:O	1:D:161:GLN:HG3	2.15	0.45
1:A:187:SER:HA	1:A:307:TYR:CE2	2.52	0.45
1:D:186:THR:OG1	1:D:187:SER:N	2.48	0.45
1:D:219:ASP:HB3	5:D:734:HOH:O	2.16	0.45
1:D:55:VAL:O	1:D:56:GLY:O	2.33	0.45
1:B:265:SER:HB3	5:B:739:HOH:O	2.16	0.45
1:A:147:GLY:HA3	1:A:152:ILE:CD1	2.45	0.45
1:C:135:PRO:O	1:C:136:THR:OG1	2.31	0.45
1:A:190:ASN:HD22	1:A:191:ASP:N	2.14	0.45
1:B:350:GLY:O	1:B:354:LYS:HG3	2.17	0.45
1:A:37:LEU:HD13	1:A:37:LEU:C	2.37	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ASN:CG	5:C:463:HOH:O	2.55	0.45
1:C:319:ASN:HD22	1:C:319:ASN:N	2.15	0.45
1:D:106:VAL:O	1:D:137:ASN:HA	2.17	0.45
1:D:280:THR:HG22	1:D:281:GLU:HG3	1.99	0.45
1:D:50:PHE:CE1	1:D:82:THR:HG23	2.52	0.45
1:A:249:LYS:H	1:A:249:LYS:HG3	1.47	0.44
1:C:94:SER:O	1:C:118:LYS:HE3	2.17	0.44
1:A:141:TYR:HB3	1:A:351:ASP:CG	2.38	0.44
1:C:147:GLY:HA3	1:C:152:ILE:HD12	1.98	0.44
1:C:265:SER:HA	1:C:268:ASP:OD2	2.17	0.44
1:A:108:ASN:N	1:A:108:ASN:ND2	2.64	0.44
1:B:173:PHE:HB3	1:B:223:LYS:HD2	1.98	0.44
1:B:2:SER:HB2	1:B:30:THR:C	2.37	0.44
1:B:311:PHE:HA	1:B:314:LEU:HD13	1.98	0.44
1:A:142:HIS:CE1	1:A:157:ARG:HH21	2.30	0.44
1:A:190:ASN:HD22	1:A:190:ASN:C	2.20	0.44
1:D:73:LEU:HD12	1:D:101:PHE:CD2	2.52	0.44
1:D:15:VAL:HB	3:D:1300:NDA:O1N	2.17	0.44
1:A:16:VAL:HG23	1:A:17:GLY:N	2.31	0.44
1:B:194:PHE:O	1:B:198:VAL:HG23	2.17	0.44
1:B:281:GLU:HB2	1:B:283:LYS:HE3	1.99	0.44
1:D:141:TYR:HB3	1:D:351:ASP:CG	2.37	0.44
1:B:315:LYS:O	1:B:316:GLY:O	2.35	0.44
1:C:353:ILE:O	1:C:357:GLN:HG3	2.18	0.44
1:A:177:LEU:HD21	1:A:215:LEU:HD23	2.00	0.43
1:B:280:THR:C	1:B:281:GLU:O	2.50	0.43
1:A:351:ASP:HA	1:A:354:LYS:HE3	2.00	0.43
1:C:164:ASP:OD1	1:C:327:ARG:HG3	2.18	0.43
1:C:42:GLU:CD	1:C:42:GLU:H	2.21	0.43
1:D:172:ILE:HD11	1:D:286:ARG:HD3	1.99	0.43
1:A:219:ASP:OD1	1:A:223:LYS:HE3	2.18	0.43
1:A:40:GLU:HB3	1:A:41:ALA:H	1.51	0.43
1:B:195:SER:O	1:B:199:LYS:HG3	2.18	0.43
1:D:304:LYS:HE2	5:D:709:HOH:O	2.18	0.43
1:D:314:LEU:HB3	1:D:318:ASP:HB3	2.00	0.43
1:B:202:LYS:NZ	1:B:209:PRO:O	2.44	0.43
1:C:210:ASP:OD1	1:C:212:ARG:HB2	2.18	0.43
1:D:83:SER:HA	1:D:84:PRO:HD3	1.78	0.43
1:B:134:LYS:HB2	1:B:137:ASN:ND2	2.33	0.43
1:D:286:ARG:HB3	1:D:286:ARG:CZ	2.47	0.43
1:A:195:SER:OG	1:A:265:SER:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:SER:HB3	1:A:98:ILE:HG12	2.01	0.43
1:C:321:ILE:HG22	1:C:323:ILE:HG13	2.01	0.43
1:A:31:ILE:CG2	1:A:32:THR:N	2.81	0.43
1:B:265:SER:HA	1:B:268:ASP:OD2	2.19	0.43
1:D:194:PHE:O	1:D:198:VAL:HG23	2.18	0.43
1:B:81:LYS:HD3	1:B:108:ASN:HB3	2.01	0.43
1:B:83:SER:HA	1:B:84:PRO:HD3	1.76	0.43
1:D:43:ARG:HH11	1:D:43:ARG:CB	2.31	0.43
1:A:166:VAL:O	1:A:293:VAL:HG21	2.18	0.43
1:B:243:VAL:CG2	1:B:243:VAL:O	2.67	0.43
1:D:236:GLU:HB3	1:D:240:SER:CB	2.49	0.43
1:D:314:LEU:HD13	1:D:318:ASP:O	2.18	0.43
1:A:134:LYS:CG	1:A:137:ASN:ND2	2.82	0.42
1:A:330:ASN:HA	1:A:330:ASN:HD22	1.61	0.42
1:B:253:SER:O	1:B:254:VAL:O	2.36	0.42
1:C:188:GLN:OE1	1:C:188:GLN:HA	2.19	0.42
1:A:30:THR:CG2	1:A:31:ILE:H	2.31	0.42
1:D:43:ARG:HG2	1:D:66:SER:O	2.20	0.42
1:A:251:LEU:HB3	1:A:260:PHE:HD1	1.84	0.42
1:A:358:ARG:O	1:A:359:LEU:HB2	2.18	0.42
1:D:152:ILE:HD12	1:D:321:ILE:CG2	2.46	0.42
1:D:212:ARG:HH11	1:D:212:ARG:CG	2.33	0.42
1:D:166:VAL:HA	1:D:325:THR:HG22	2.01	0.42
1:D:43:ARG:HB2	1:D:43:ARG:CZ	2.50	0.42
1:A:2:SER:HB3	1:A:359:LEU:OXT	2.19	0.42
1:D:187:SER:HA	1:D:307:TYR:CE2	2.54	0.42
1:B:210:ASP:HB3	1:B:213:ASP:OD1	2.20	0.42
1:C:173:PHE:CD1	1:C:173:PHE:N	2.88	0.42
1:C:176:THR:O	1:C:180:ILE:HG13	2.19	0.42
1:D:315:LYS:HA	5:D:516:HOH:O	2.19	0.42
1:A:81:LYS:CB	1:A:81:LYS:NZ	2.81	0.42
1:B:236:GLU:O	1:B:237:SER:HB3	2.19	0.42
1:B:36:VAL:CG1	1:B:36:VAL:O	2.68	0.42
1:A:254:VAL:O	1:A:255:LYS:HB3	2.19	0.42
1:A:256:SER:HB2	1:A:259:GLU:HG3	2.02	0.42
1:D:179:TYR:HA	1:D:316:GLY:O	2.20	0.42
1:A:184:PHE:CE2	1:A:275:LYS:HD3	2.55	0.42
1:A:349:LEU:HB3	1:B:162:THR:HG22	2.01	0.42
1:B:300:VAL:HG23	1:B:300:VAL:O	2.20	0.42
1:B:72:PRO:O	1:B:75:ASP:N	2.53	0.42
1:C:134:LYS:HB2	1:C:137:ASN:ND2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:LEU:H	1:C:251:LEU:CD1	2.33	0.42
1:D:121:SER:CB	1:D:222:ARG:HB3	2.50	0.42
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.67	0.41
1:B:153:ILE:N	1:B:153:ILE:CD1	2.83	0.41
1:B:36:VAL:HG12	1:B:36:VAL:O	2.20	0.41
1:C:123:ASP:OD2	1:C:125:ALA:HB3	2.19	0.41
1:C:335:GLN:HG2	1:D:333:VAL:HB	2.02	0.41
1:A:198:VAL:CG2	1:A:199:LYS:N	2.84	0.41
1:D:190:ASN:OD1	1:D:191:ASP:N	2.53	0.41
1:A:18:SER:HB3	5:A:487:HOH:O	2.19	0.41
1:B:116:ASN:HD22	1:B:116:ASN:C	2.22	0.41
1:A:254:VAL:O	1:A:255:LYS:CB	2.68	0.41
1:B:2:SER:HB3	1:B:31:ILE:HA	2.03	0.41
1:C:152:ILE:HG21	1:C:321:ILE:CD1	2.50	0.41
1:C:275:LYS:HA	1:C:285:LEU:HD11	2.01	0.41
1:A:281:GLU:O	1:A:282:ASN:HB2	2.20	0.41
1:C:327:ARG:HD2	5:C:736:HOH:O	2.20	0.41
1:D:212:ARG:HH21	1:D:254:VAL:HG23	1.81	0.41
1:A:142:HIS:HD2	1:A:145:THR:OG1	2.03	0.41
1:A:263:LYS:HG3	1:A:263:LYS:O	2.21	0.41
1:A:139:PHE:CE2	1:A:358:ARG:NH2	2.89	0.41
1:A:38:LEU:HD21	1:A:63:LEU:HD22	2.01	0.41
1:A:134:LYS:HB2	1:A:137:ASN:CG	2.41	0.41
1:A:256:SER:CB	1:A:259:GLU:HG3	2.51	0.41
1:A:198:VAL:HG23	1:A:199:LYS:N	2.36	0.40
1:B:124:LEU:O	1:B:128:LYS:HG2	2.21	0.40
1:B:304:LYS:NZ	1:B:304:LYS:CB	2.82	0.40
1:B:309:HIS:CG	1:B:310:PRO:HD2	2.56	0.40
1:A:328:TYR:OH	1:B:343:VAL:HG13	2.21	0.40
1:D:219:ASP:HB2	5:D:640:HOH:O	2.21	0.40
1:C:134:LYS:HA	1:C:135:PRO:HD3	1.98	0.40
1:C:157:ARG:O	1:C:161:GLN:HG3	2.21	0.40
1:C:30:THR:CG2	1:C:31:ILE:N	2.82	0.40
1:A:77:ILE:O	1:A:81:LYS:HG3	2.21	0.40
1:C:153:ILE:O	1:C:157:ARG:HG2	2.20	0.40
1:C:254:VAL:HG21	1:C:260:PHE:HB2	2.03	0.40
1:C:83:SER:HA	1:C:84:PRO:HD3	1.88	0.40
1:D:93:THR:O	1:D:116:ASN:HB2	2.21	0.40
1:B:247:ILE:HA	1:B:248:PRO:HD3	1.95	0.40
1:C:166:VAL:HG23	5:C:665:HOH:O	2.21	0.40
1:C:204:LEU:HB2	1:C:206:TYR:CD1	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:HG22	1:A:32:THR:N	2.36	0.40
1:C:142:HIS:HB2	1:C:145:THR:HG21	2.03	0.40
1:D:145:THR:CG2	1:D:226:ILE:CD1	2.99	0.40
1:D:281:GLU:O	1:D:283:LYS:HG3	2.21	0.40
1:D:330:ASN:HA	1:D:331:PRO:HD3	1.94	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	356/358 (99%)	320 (90%)	27 (8%)	9 (2%)	6	11
1	B	356/358 (99%)	322 (90%)	30 (8%)	4 (1%)	17	35
1	C	356/358 (99%)	322 (90%)	30 (8%)	4 (1%)	17	35
1	D	356/358 (99%)	326 (92%)	27 (8%)	3 (1%)	22	44
All	All	1424/1432 (99%)	1290 (91%)	114 (8%)	20 (1%)	13	26

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ALA
1	B	254	VAL
1	B	279	ALA
1	C	41	ALA
1	D	234	GLU
1	A	3	THR
1	A	265	SER
1	B	234	GLU
1	B	316	GLY
1	C	136	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	316	GLY
1	D	56	GLY
1	D	253	SER
1	A	255	LYS
1	A	189	ALA
1	A	234	GLU
1	A	249	LYS
1	A	250	PRO
1	A	211	PRO
1	C	250	PRO

5.3.2 Protein sidechains ⓘ

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	300/300 (100%)	289 (96%)	11 (4%)	39	66
1	B	300/300 (100%)	284 (95%)	16 (5%)	26	50
1	C	300/300 (100%)	292 (97%)	8 (3%)	50	77
1	D	300/300 (100%)	287 (96%)	13 (4%)	33	61
All	All	1200/1200 (100%)	1152 (96%)	48 (4%)	36	64

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	42	GLU
1	A	46	ILE
1	A	108	ASN
1	A	123	ASP
1	A	190	ASN
1	A	212	ARG
1	A	256	SER
1	A	267	TYR
1	A	303	GLU
1	A	306	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	54	ASN
1	B	57	SER
1	B	58	ASP
1	B	94	SER
1	B	116	ASN
1	B	157	ARG
1	B	212	ARG
1	B	243	VAL
1	B	270	ASP
1	B	271	LEU
1	B	280	THR
1	B	282	ASN
1	B	304	LYS
1	B	319	ASN
1	B	320	VAL
1	B	329	THR
1	C	4	LYS
1	C	28	LYS
1	C	190	ASN
1	C	212	ARG
1	C	297	SER
1	C	303	GLU
1	C	306	ASP
1	C	308	SER
1	D	94	SER
1	D	116	ASN
1	D	157	ARG
1	D	186	THR
1	D	191	ASP
1	D	197	VAL
1	D	212	ARG
1	D	240	SER
1	D	243	VAL
1	D	280	THR
1	D	303	GLU
1	D	304	LYS
1	D	324	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	108	ASN
1	A	133	ASN
1	A	142	HIS
1	A	190	ASN
1	A	309	HIS
1	A	319	ASN
1	A	330	ASN
1	B	92	ASN
1	B	116	ASN
1	B	133	ASN
1	B	137	ASN
1	B	188	GLN
1	B	190	ASN
1	B	309	HIS
1	B	319	ASN
1	B	330	ASN
1	C	7	ASN
1	C	133	ASN
1	C	142	HIS
1	C	161	GLN
1	C	190	ASN
1	C	309	HIS
1	C	330	ASN
1	D	116	ASN
1	D	137	ASN
1	D	182	ASN
1	D	188	GLN
1	D	330	ASN
1	D	335	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

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	NDA	D	1300	-	40,47,47	2.00	6 (15%)	41,71,71	1.38	4 (9%)
4	HSE	D	1301	-	2,7,7	0.38	0	1,8,8	0.39	0

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
3	NDA	D	1300	-	-	0/20/60/60	0/5/5/5
4	HSE	D	1301	-	-	0/3/7/7	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1300	NDA	C6N-C5N	-2.46	1.33	1.38
3	D	1300	NDA	C2A-N1A	2.52	1.38	1.33
3	D	1300	NDA	C6N-N1N	3.47	1.44	1.35
3	D	1300	NDA	C5N-C4N	5.54	1.49	1.38
3	D	1300	NDA	C4N-C3N	6.45	1.52	1.38
3	D	1300	NDA	C2N-C3N	6.71	1.51	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1300	NDA	C5N-C4N-C3N	-5.06	112.93	120.64
3	D	1300	NDA	O2N-PN-O5D	2.06	117.86	108.14
3	D	1300	NDA	C5A-C6A-N6A	2.40	125.36	120.47
3	D	1300	NDA	C6N-C5N-C4N	4.09	125.62	119.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1300	NDA	3	0
4	D	1301	HSE	1	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, 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	358/358 (100%)	-0.18	11 (3%) 49 41	9, 25, 72, 94	0
1	B	358/358 (100%)	-0.37	1 (0%) 93 93	8, 22, 56, 83	0
1	C	358/358 (100%)	-0.25	6 (1%) 70 65	8, 25, 66, 93	0
1	D	358/358 (100%)	-0.45	2 (0%) 89 88	7, 22, 42, 75	0
All	All	1432/1432 (100%)	-0.31	20 (1%) 75 71	7, 23, 58, 94	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	SER	5.0
1	A	189	ALA	4.9
1	A	133	ASN	4.3
1	A	191	ASP	4.0
1	C	2	SER	3.7
1	C	3	THR	3.6
1	A	188	GLN	3.6
1	B	2	SER	3.6
1	A	190	ASN	3.4
1	C	255	LYS	2.8
1	C	279	ALA	2.7
1	C	188	GLN	2.5
1	C	189	ALA	2.5
1	A	135	PRO	2.4
1	A	257	ALA	2.3
1	A	3	THR	2.3
1	D	3	THR	2.3
1	A	249	LYS	2.1
1	A	252	GLU	2.1
1	A	125	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, 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
3	NDA	D	1300	43/43	0.74	0.34	9.65	46,66,83,91	0
4	HSE	D	1301	8/8	0.67	0.33	7.07	43,50,61,61	0
2	NA	A	901	1/1	0.89	0.24	2.41	24,24,24,24	0
2	NA	C	903	1/1	0.88	0.17	1.20	22,22,22,22	0
2	NA	B	902	1/1	0.93	0.13	-0.31	21,21,21,21	0
2	NA	D	904	1/1	0.94	0.08	-4.19	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.