Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 04:37 PM EDT

PDB ID	:	4NSL
Title	:	X-ray Crystal structure of Adenylosuccinate Lyase from Salmonella typhimurium
Authors	:	Banerjee, S.; Agrawal, M.J.; Murthy, M.R.N.
Deposited on	:	2013-11-28
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

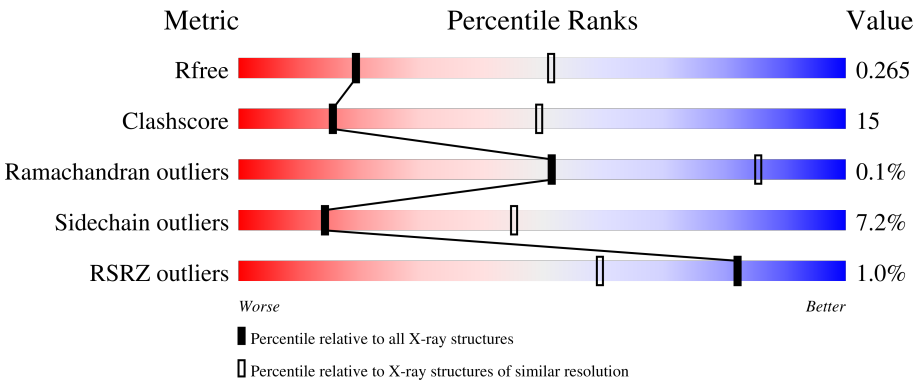
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	470	% 59% 34% • 5%
1	B	470	% 64% 30% • 5%
1	C	470	% 63% 29% • 5%
1	D	470	% 64% 29% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14068 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 Adenylosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3527	2251	608	658	10	0	0	0
1	B	447	3489	2227	603	650	9	0	0	0
1	C	446	3513	2245	602	657	9	0	0	0
1	D	443	3486	2225	603	649	9	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q8ZPZ6
A	-12	ARG	-	expression tag	UNP Q8ZPZ6
A	-11	GLY	-	expression tag	UNP Q8ZPZ6
A	-10	SER	-	expression tag	UNP Q8ZPZ6
A	-9	HIS	-	expression tag	UNP Q8ZPZ6
A	-8	HIS	-	expression tag	UNP Q8ZPZ6
A	-7	HIS	-	expression tag	UNP Q8ZPZ6
A	-6	HIS	-	expression tag	UNP Q8ZPZ6
A	-5	HIS	-	expression tag	UNP Q8ZPZ6
A	-4	HIS	-	expression tag	UNP Q8ZPZ6
A	-3	GLY	-	expression tag	UNP Q8ZPZ6
A	-2	MET	-	expression tag	UNP Q8ZPZ6
A	-1	ALA	-	expression tag	UNP Q8ZPZ6
A	0	SER	-	expression tag	UNP Q8ZPZ6
B	-13	MET	-	initiating methionine	UNP Q8ZPZ6
B	-12	ARG	-	expression tag	UNP Q8ZPZ6
B	-11	GLY	-	expression tag	UNP Q8ZPZ6
B	-10	SER	-	expression tag	UNP Q8ZPZ6
B	-9	HIS	-	expression tag	UNP Q8ZPZ6
B	-8	HIS	-	expression tag	UNP Q8ZPZ6
B	-7	HIS	-	expression tag	UNP Q8ZPZ6

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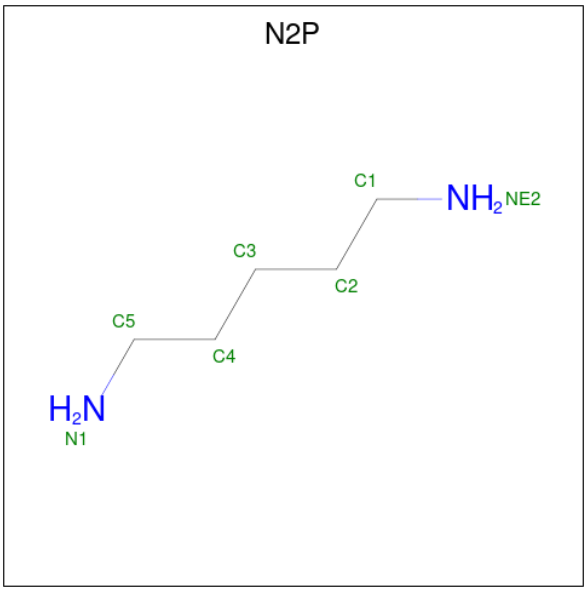
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q8ZPZ6
B	-5	HIS	-	expression tag	UNP Q8ZPZ6
B	-4	HIS	-	expression tag	UNP Q8ZPZ6
B	-3	GLY	-	expression tag	UNP Q8ZPZ6
B	-2	MET	-	expression tag	UNP Q8ZPZ6
B	-1	ALA	-	expression tag	UNP Q8ZPZ6
B	0	SER	-	expression tag	UNP Q8ZPZ6
C	-13	MET	-	initiating methionine	UNP Q8ZPZ6
C	-12	ARG	-	expression tag	UNP Q8ZPZ6
C	-11	GLY	-	expression tag	UNP Q8ZPZ6
C	-10	SER	-	expression tag	UNP Q8ZPZ6
C	-9	HIS	-	expression tag	UNP Q8ZPZ6
C	-8	HIS	-	expression tag	UNP Q8ZPZ6
C	-7	HIS	-	expression tag	UNP Q8ZPZ6
C	-6	HIS	-	expression tag	UNP Q8ZPZ6
C	-5	HIS	-	expression tag	UNP Q8ZPZ6
C	-4	HIS	-	expression tag	UNP Q8ZPZ6
C	-3	GLY	-	expression tag	UNP Q8ZPZ6
C	-2	MET	-	expression tag	UNP Q8ZPZ6
C	-1	ALA	-	expression tag	UNP Q8ZPZ6
C	0	SER	-	expression tag	UNP Q8ZPZ6
D	-13	MET	-	initiating methionine	UNP Q8ZPZ6
D	-12	ARG	-	expression tag	UNP Q8ZPZ6
D	-11	GLY	-	expression tag	UNP Q8ZPZ6
D	-10	SER	-	expression tag	UNP Q8ZPZ6
D	-9	HIS	-	expression tag	UNP Q8ZPZ6
D	-8	HIS	-	expression tag	UNP Q8ZPZ6
D	-7	HIS	-	expression tag	UNP Q8ZPZ6
D	-6	HIS	-	expression tag	UNP Q8ZPZ6
D	-5	HIS	-	expression tag	UNP Q8ZPZ6
D	-4	HIS	-	expression tag	UNP Q8ZPZ6
D	-3	GLY	-	expression tag	UNP Q8ZPZ6
D	-2	MET	-	expression tag	UNP Q8ZPZ6
D	-1	ALA	-	expression tag	UNP Q8ZPZ6
D	0	SER	-	expression tag	UNP Q8ZPZ6

- Molecule 2 is PENTANE-1,5-DIAMINE (three-letter code: N2P) (formula: $C_5H_{14}N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	B	1	7	5	2	0	0
2	C	1	7	5	2	0	0

- Molecule 3 is water.

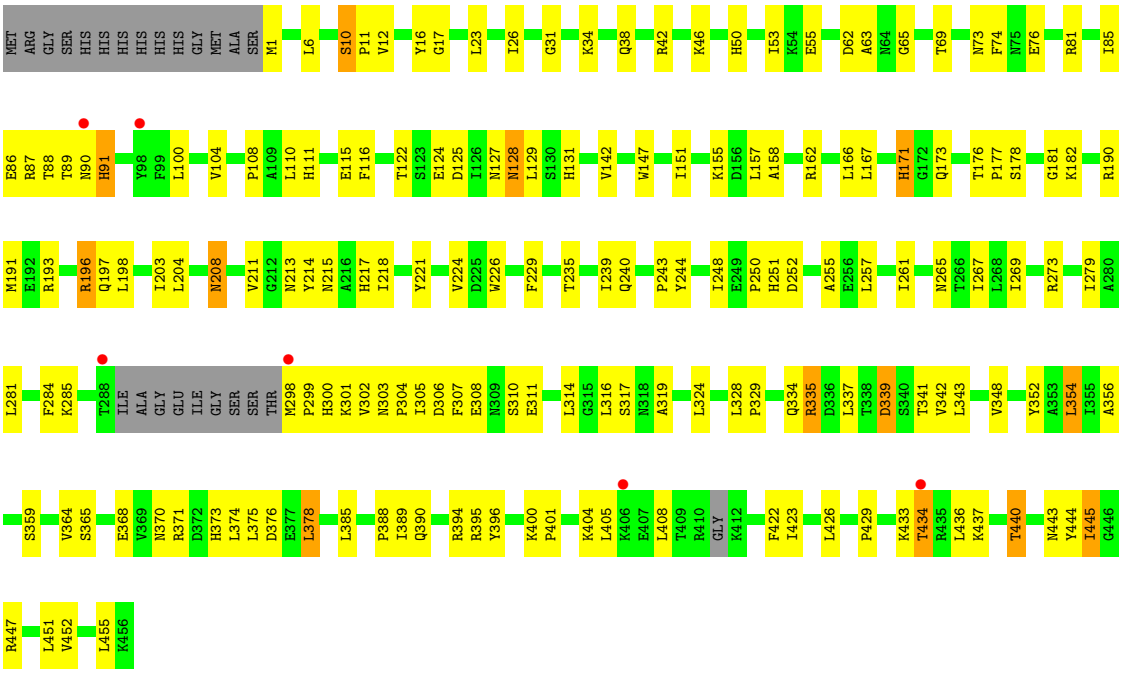
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	10	10	10	0	0
3	B	11	11	11	0	0
3	C	8	8	8	0	0
3	D	10	10	10	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

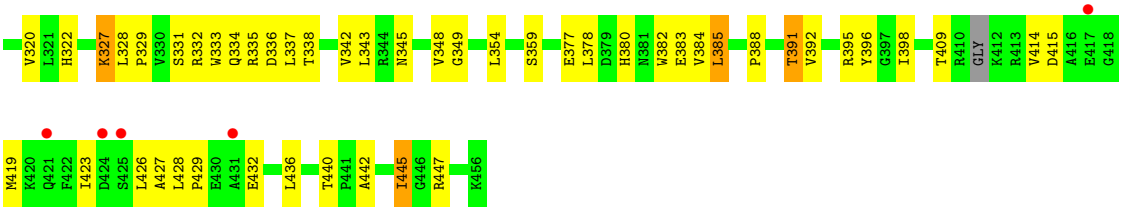
• Molecule 1: Adenylosuccinate lyase

Chain A:



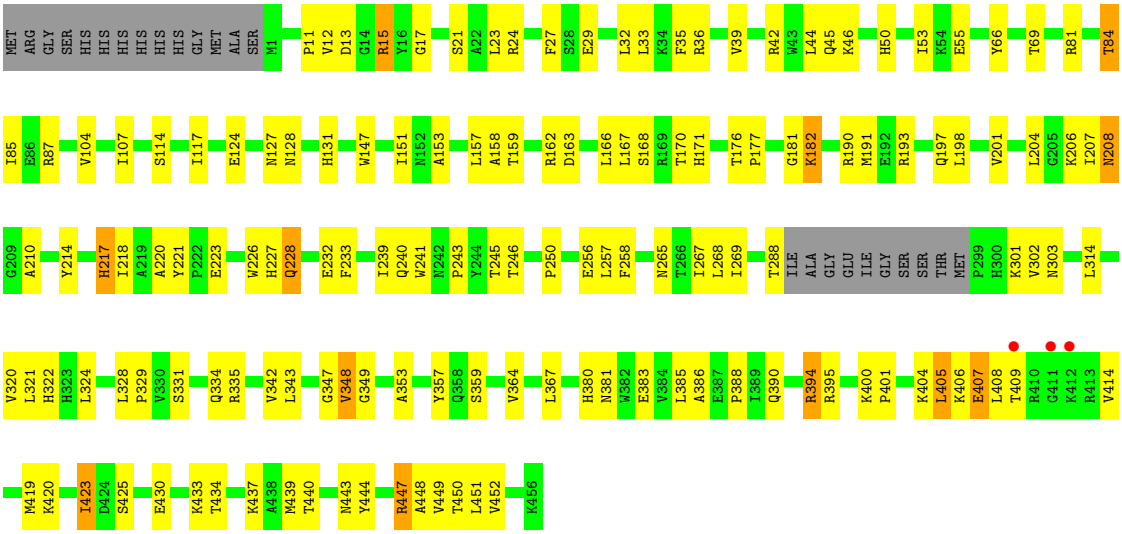
• Molecule 1: Adenylosuccinate lyase

Chain B:



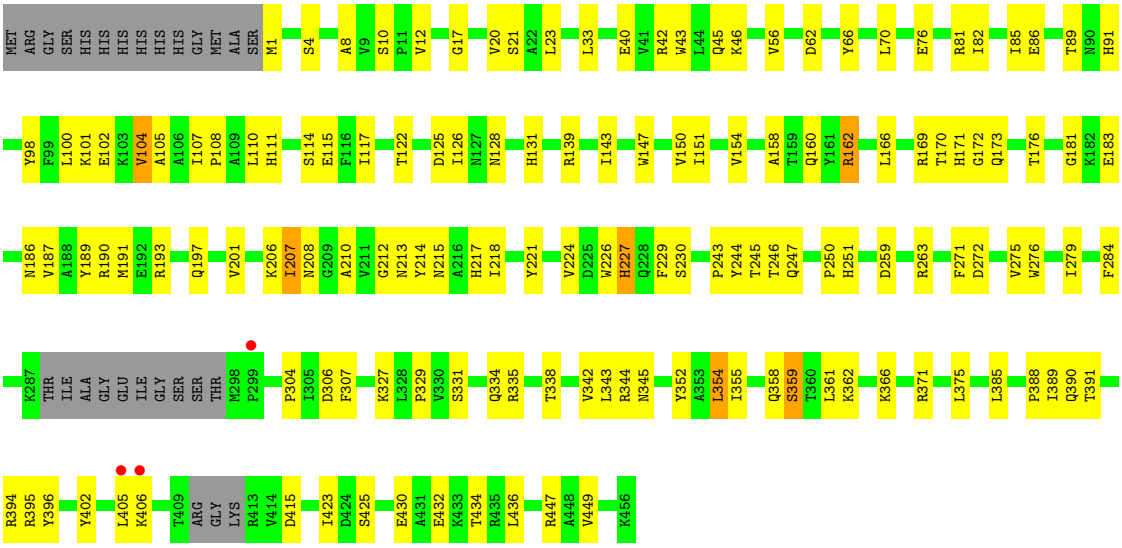
• Molecule 1: Adenylosuccinate lyase

Chain C:



• Molecule 1: Adenylosuccinate lyase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.71Å 102.30Å 198.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.61 – 3.00 34.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (33.61-3.00) 97.5 (34.09-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.220 , 0.274 0.211 , 0.265	Depositor DCC
R_{free} test set	1780 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14068	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: N2P

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	0.24	0/3603	0.43	0/4900
1	B	0.24	0/3562	0.43	0/4843
1	C	0.25	0/3590	0.45	0/4884
1	D	0.24	0/3561	0.42	0/4843
All	All	0.24	0/14316	0.43	0/19470

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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	206	LYS	Peptide
1	D	206	LYS	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	3527	0	3446	138	0
1	B	3489	0	3397	109	0
1	C	3513	0	3429	102	0
1	D	3486	0	3405	94	0
2	B	7	0	14	0	0
2	C	7	0	14	0	0
3	A	10	0	0	0	0
3	B	11	0	0	1	0
3	C	8	0	0	0	0
3	D	10	0	0	0	0
All	All	14068	0	13705	411	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 15.

All (411) 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:206:LYS:HD3	1:C:207:ILE:H	1.33	0.93
1:D:208:ASN:HD21	1:D:245:THR:HB	1.33	0.92
1:D:208:ASN:ND2	1:D:245:THR:HB	1.88	0.88
1:C:388:PRO:HG3	1:C:444:TYR:CZ	2.11	0.86
1:B:179:THR:HG23	1:B:445:ILE:HG21	1.60	0.84
1:D:125:ASP:HB3	1:D:207:ILE:HG22	1.59	0.84
1:A:239:ILE:HG22	1:A:240:GLN:H	1.43	0.83
1:B:208:ASN:HB3	1:B:212:GLY:HA2	1.60	0.82
1:C:423:ILE:HD11	1:C:437:LYS:HG3	1.59	0.82
1:C:245:THR:HG22	1:C:246:THR:O	1.85	0.77
1:C:405:LEU:C	1:C:407:GLU:H	1.90	0.75
1:D:402:TYR:O	1:D:406:LYS:HB2	1.87	0.75
1:B:208:ASN:CB	1:B:212:GLY:HA2	2.15	0.74
1:C:206:LYS:HD3	1:C:207:ILE:N	2.03	0.74
1:B:427:ALA:O	1:B:428:LEU:HD12	1.88	0.73
1:C:13:ASP:OD2	1:D:8:ALA:HB1	1.88	0.73
1:A:104:VAL:CG1	1:A:110:LEU:HB2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ASP:HB3	1:B:207:ILE:HG22	1.69	0.72
1:B:239:ILE:HG22	1:B:240:GLN:H	1.54	0.72
1:A:142:VAL:HG11	1:A:354:LEU:HD11	1.72	0.72
1:C:258:PHE:HB3	1:C:321:LEU:HB3	1.73	0.70
1:D:89:THR:HG23	1:D:91:HIS:H	1.54	0.69
1:B:47:LEU:C	1:B:53:ILE:HD11	2.12	0.69
1:C:15:ARG:HD3	1:D:344:ARG:CZ	2.23	0.69
1:C:239:ILE:HG22	1:C:240:GLN:H	1.58	0.69
1:A:279:ILE:HD13	1:A:304:PRO:HB3	1.74	0.69
1:A:324:LEU:HD22	1:A:342:VAL:HG13	1.75	0.69
1:C:334:GLN:O	1:C:335:ARG:HB3	1.93	0.68
1:A:451:LEU:HD21	1:D:227:HIS:CE1	2.28	0.68
1:A:370:ASN:O	1:A:374:LEU:HD13	1.94	0.68
1:C:44:LEU:HD22	1:C:117:ILE:HG12	1.76	0.67
1:B:335:ARG:HG2	1:B:336:ASP:N	2.09	0.67
1:A:63:ALA:HB1	1:A:110:LEU:HD21	1.77	0.66
1:B:161:TYR:HA	1:B:164:ILE:HD12	1.78	0.66
1:B:53:ILE:O	1:B:53:ILE:HG13	1.95	0.66
1:A:440:THR:H	1:A:443:ASN:HB3	1.60	0.66
1:C:50:HIS:HB3	1:C:53:ILE:HD12	1.77	0.66
1:A:300:HIS:NE2	1:C:409:THR:HG22	2.10	0.66
1:A:305:ILE:HD12	1:B:337:LEU:HD22	1.77	0.65
1:A:390:GLN:HG2	1:A:405:LEU:CD1	2.27	0.65
1:A:100:LEU:O	1:A:104:VAL:HG23	1.97	0.64
1:B:107:ILE:HD12	1:B:110:LEU:HD12	1.77	0.64
1:B:53:ILE:HG22	1:B:221:TYR:CE1	2.32	0.64
1:A:303:ASN:OD1	1:A:305:ILE:HG12	1.97	0.64
1:A:423:ILE:HG21	1:A:437:LYS:HG3	1.79	0.64
1:B:63:ALA:HB1	1:B:110:LEU:HD21	1.80	0.63
1:A:390:GLN:HG2	1:A:405:LEU:HD13	1.78	0.63
1:D:101:LYS:HG2	1:D:117:ILE:HD12	1.81	0.63
1:A:335:ARG:NH2	1:A:337:LEU:HG	2.14	0.63
1:D:98:TYR:O	1:D:102:GLU:HB2	1.98	0.62
1:A:423:ILE:HA	1:A:426:LEU:HD12	1.79	0.62
1:A:314:LEU:O	1:A:317:SER:HB3	1.98	0.62
1:B:334:GLN:O	1:B:335:ARG:HB2	1.98	0.62
1:C:388:PRO:HB2	1:C:439:MET:HE1	1.81	0.62
1:A:281:LEU:O	1:A:373:HIS:HE1	1.82	0.62
1:B:398:ILE:HD11	1:B:428:LEU:HD12	1.81	0.62
1:C:320:VAL:HG11	1:C:348:VAL:HG12	1.82	0.61
1:B:47:LEU:O	1:B:53:ILE:HD11	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ILE:HG12	1:A:191:MET:HB3	1.83	0.60
1:A:248:ILE:HG23	1:A:335:ARG:HD2	1.83	0.60
1:B:314:LEU:O	1:B:317:SER:HB3	2.02	0.60
1:C:419:MET:O	1:C:423:ILE:HG23	2.01	0.60
1:B:198:LEU:O	1:B:201:VAL:HG12	2.02	0.60
1:B:44:LEU:HD22	1:B:117:ILE:HG12	1.83	0.59
1:C:207:ILE:HG23	1:C:207:ILE:O	2.01	0.59
1:C:162:ARG:HA	1:C:181:GLY:HA3	1.85	0.59
1:D:86:GLU:HA	1:D:89:THR:HG22	1.84	0.59
1:D:208:ASN:HA	1:D:214:TYR:CE1	2.37	0.59
1:B:43:TRP:CZ3	1:B:207:ILE:HD13	2.37	0.59
1:C:420:LYS:HG3	1:C:437:LYS:HD3	1.83	0.59
1:B:55:GLU:HB3	1:B:116:PHE:CZ	2.36	0.59
1:A:50:HIS:HB3	1:A:53:ILE:HD13	1.85	0.58
1:A:248:ILE:CG2	1:A:335:ARG:HH11	2.16	0.58
1:A:162:ARG:HB2	1:A:452:VAL:HG11	1.85	0.58
1:A:440:THR:HG23	1:A:443:ASN:HB2	1.86	0.58
1:B:207:ILE:HD11	1:B:230:SER:HA	1.86	0.58
1:C:383:GLU:HG3	1:C:414:VAL:HG21	1.85	0.58
1:B:118:HIS:O	1:B:118:HIS:CD2	2.56	0.58
1:B:167:LEU:N	1:B:378:LEU:HD11	2.18	0.58
1:C:35:PHE:O	1:C:39:VAL:HG12	2.04	0.58
1:A:104:VAL:CG1	1:A:110:LEU:CB	2.81	0.57
1:C:221:TYR:HB2	1:C:226:TRP:HZ2	1.69	0.57
1:C:84:THR:HA	1:C:87:ARG:HD2	1.86	0.57
1:C:66:TYR:O	1:C:69:THR:HG22	2.04	0.57
1:B:345:ASN:O	1:B:348:VAL:HG22	2.03	0.57
1:A:151:ILE:HG22	1:A:155:LYS:HE2	1.86	0.57
1:A:190:ARG:HB3	1:A:267:ILE:HD13	1.85	0.57
1:C:158:ALA:HA	1:C:181:GLY:HA2	1.86	0.57
1:B:334:GLN:HG2	1:C:168:SER:HB3	1.86	0.56
1:C:385:LEU:O	1:C:388:PRO:HD2	2.05	0.56
1:B:12:VAL:O	1:B:17:GLY:HA2	2.04	0.56
1:A:455:LEU:HD12	1:D:244:TYR:CZ	2.40	0.56
1:C:250:PRO:O	1:C:329:PRO:HA	2.05	0.56
1:D:334:GLN:O	1:D:335:ARG:HB3	2.05	0.56
1:A:221:TYR:HB2	1:A:226:TRP:HZ2	1.71	0.56
1:C:405:LEU:C	1:C:407:GLU:N	2.58	0.56
1:B:55:GLU:O	1:B:57:PRO:HD3	2.07	0.55
1:C:167:LEU:HD22	1:C:381:ASN:ND2	2.21	0.55
1:A:53:ILE:N	1:A:53:ILE:HD12	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:PHE:HE1	1:C:394:ARG:HB3	1.70	0.55
1:B:250:PRO:O	1:B:329:PRO:HA	2.07	0.55
1:A:269:ILE:HG23	1:A:311:GLU:HG3	1.89	0.55
1:B:167:LEU:HD21	1:B:174:PRO:HB3	1.89	0.55
1:C:388:PRO:HG3	1:C:444:TYR:OH	2.05	0.55
1:C:239:ILE:HG22	1:C:240:GLN:N	2.22	0.55
1:B:310:SER:HB2	1:B:359:SER:HB2	1.88	0.55
1:C:157:LEU:HD21	1:C:367:LEU:HD12	1.89	0.54
1:D:389:ILE:HG12	1:D:436:LEU:HD22	1.89	0.54
1:B:378:LEU:HD23	1:B:442:ALA:HA	1.89	0.54
1:A:211:VAL:HG11	1:D:176:THR:O	2.08	0.54
1:D:33:LEU:HD22	1:D:82:ILE:HG21	1.88	0.54
1:A:239:ILE:HG22	1:A:240:GLN:N	2.20	0.54
1:A:423:ILE:O	1:A:433:LYS:HE2	2.08	0.54
1:B:239:ILE:HG22	1:B:240:GLN:N	2.22	0.54
1:A:86:GLU:C	1:A:88:THR:H	2.11	0.54
1:C:182:LYS:HE3	1:C:451:LEU:HD13	1.90	0.54
1:A:273:ARG:HG2	1:B:332:ARG:HH21	1.74	0.53
1:C:167:LEU:HD22	1:C:381:ASN:HD22	1.73	0.53
1:A:400:LYS:N	1:A:401:PRO:HD3	2.23	0.53
1:B:43:TRP:HZ3	1:B:207:ILE:HD13	1.74	0.53
1:A:46:LYS:HG2	1:A:229:PHE:CZ	2.44	0.53
1:A:89:THR:C	1:A:91:HIS:H	2.11	0.53
1:A:248:ILE:CG2	1:A:335:ARG:HD2	2.39	0.53
1:A:182:LYS:NZ	1:A:451:LEU:HD13	2.24	0.52
1:A:447:ARG:HB2	1:D:218:ILE:HD11	1.89	0.52
1:B:208:ASN:HB3	1:B:212:GLY:CA	2.36	0.52
1:B:327:LYS:HE3	1:B:342:VAL:HG21	1.91	0.52
1:D:40:GLU:OE2	1:D:126:ILE:HG13	2.09	0.52
1:B:243:PRO:HG2	1:B:244:TYR:HD2	1.75	0.52
1:C:124:GLU:HA	1:C:127:ASN:HB2	1.90	0.52
1:A:279:ILE:HG12	1:A:302:VAL:HG13	1.91	0.52
1:C:386:ALA:O	1:C:390:GLN:OE1	2.28	0.52
1:D:158:ALA:HA	1:D:181:GLY:HA2	1.91	0.52
1:A:334:GLN:O	1:A:335:ARG:HB3	2.09	0.52
1:C:81:ARG:O	1:C:85:ILE:HG13	2.10	0.52
1:B:161:TYR:HB3	1:B:180:LEU:HB2	1.91	0.51
1:D:243:PRO:HG2	1:D:244:TYR:CD2	2.46	0.51
1:C:401:PRO:O	1:C:405:LEU:HD12	2.10	0.51
1:D:423:ILE:HD13	1:D:436:LEU:HB3	1.93	0.51
1:A:81:ARG:O	1:A:85:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ARG:HB2	1:C:218:ILE:HD11	1.93	0.51
1:A:124:GLU:HA	1:A:127:ASN:HB2	1.93	0.51
1:A:23:LEU:HD11	1:A:354:LEU:HD13	1.92	0.51
1:D:104:VAL:HG22	1:D:110:LEU:HD13	1.92	0.51
1:A:444:TYR:CZ	1:D:215:ASN:HB3	2.46	0.51
1:A:208:ASN:HA	1:A:214:TYR:CE1	2.45	0.51
1:B:206:LYS:HG2	1:B:245:THR:HG21	1.93	0.51
1:B:249:GLU:HG2	1:B:250:PRO:HD2	1.93	0.51
1:C:107:ILE:HD12	1:C:107:ILE:H	1.75	0.50
1:C:241:TRP:CH2	1:C:243:PRO:HB3	2.46	0.50
1:D:217:HIS:HB3	1:D:226:TRP:CE2	2.46	0.50
1:A:10:SER:HB2	1:B:348:VAL:HG12	1.93	0.50
1:B:124:GLU:HA	1:B:127:ASN:HB2	1.92	0.50
1:C:157:LEU:HD11	1:C:364:VAL:HG13	1.94	0.50
1:D:208:ASN:HB2	1:D:212:GLY:HA2	1.93	0.50
1:C:162:ARG:HG3	1:C:163:ASP:N	2.26	0.50
1:D:170:THR:O	1:D:171:HIS:CG	2.65	0.50
1:D:12:VAL:O	1:D:17:GLY:HA2	2.12	0.50
1:D:186:ASN:O	1:D:190:ARG:HG3	2.11	0.50
1:B:183:GLU:CD	1:C:334:GLN:HE21	2.15	0.50
1:C:348:VAL:HG12	1:C:349:GLY:N	2.27	0.50
1:A:389:ILE:HG12	1:A:436:LEU:HD22	1.94	0.50
1:B:322:HIS:CE1	1:C:322:HIS:CD2	3.00	0.50
1:A:385:LEU:O	1:A:389:ILE:HG13	2.12	0.50
1:B:426:LEU:HB3	1:B:428:LEU:HD13	1.93	0.50
1:D:125:ASP:CB	1:D:207:ILE:HG22	2.38	0.50
1:B:208:ASN:HB2	1:B:212:GLY:HA2	1.92	0.50
1:C:21:SER:O	1:C:24:ARG:HB2	2.12	0.50
1:D:250:PRO:O	1:D:329:PRO:HA	2.10	0.49
1:A:388:PRO:HB3	1:A:444:TYR:CE1	2.47	0.49
1:B:249:GLU:CD	1:B:251:HIS:H	2.16	0.49
1:C:405:LEU:HD12	1:C:405:LEU:H	1.77	0.49
1:D:139:ARG:HA	1:D:143:ILE:HD12	1.94	0.49
1:A:213:ASN:HB2	1:A:215:ASN:ND2	2.26	0.49
1:C:162:ARG:HB3	1:C:452:VAL:HG11	1.94	0.49
1:C:388:PRO:CB	1:C:439:MET:HE1	2.42	0.49
1:D:66:TYR:O	1:D:70:LEU:HB2	2.12	0.49
1:D:208:ASN:CG	1:D:212:GLY:HA2	2.33	0.49
1:B:348:VAL:HG23	1:B:349:GLY:N	2.27	0.49
1:C:324:LEU:O	1:C:328:LEU:HB2	2.13	0.49
1:A:104:VAL:HG12	1:A:110:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ARG:HD3	1:A:396:TYR:CE2	2.47	0.49
1:D:221:TYR:HB2	1:D:226:TRP:HZ2	1.77	0.49
1:B:382:TRP:CH2	1:B:440:THR:HG22	2.47	0.48
1:D:104:VAL:HG22	1:D:110:LEU:HB3	1.94	0.48
1:A:193:ARG:HG2	1:A:196:ARG:NH2	2.29	0.48
1:A:217:HIS:HB3	1:A:226:TRP:CE2	2.47	0.48
1:B:33:LEU:HD23	1:B:36:ARG:HH11	1.78	0.48
1:C:444:TYR:O	1:C:444:TYR:CG	2.66	0.48
1:B:38:GLN:O	1:B:42:ARG:HG2	2.14	0.48
1:B:383:GLU:OE2	1:B:414:VAL:HG21	2.14	0.48
1:A:50:HIS:HE1	1:A:224:VAL:HG13	1.79	0.48
1:A:440:THR:H	1:A:443:ASN:CB	2.25	0.48
1:C:265:ASN:O	1:C:269:ILE:HG13	2.13	0.48
1:A:63:ALA:HB1	1:A:110:LEU:CD2	2.43	0.47
1:B:214:TYR:HD2	1:C:447:ARG:HD3	1.77	0.47
1:B:391:THR:HB	1:C:220:ALA:HB2	1.96	0.47
1:C:84:THR:O	1:C:87:ARG:HB2	2.14	0.47
1:C:439:MET:HA	1:C:443:ASN:HD21	1.79	0.47
1:D:385:LEU:C	1:D:388:PRO:HD2	2.35	0.47
1:B:147:TRP:CH2	1:B:198:LEU:HD22	2.49	0.47
1:A:408:LEU:HD12	1:A:422:PHE:HB2	1.96	0.47
1:D:208:ASN:HD21	1:D:245:THR:CB	2.14	0.47
1:D:245:THR:HG22	1:D:246:THR:O	2.14	0.47
1:A:69:THR:O	1:A:73:ASN:HB2	2.14	0.47
1:A:298:MET:HB3	1:A:299:PRO:CD	2.45	0.47
1:B:203:ILE:O	1:B:240:GLN:HB2	2.14	0.47
1:D:131:HIS:CE1	1:D:343:LEU:HD13	2.48	0.47
1:A:311:GLU:HG2	1:A:311:GLU:O	2.14	0.47
1:D:169:ARG:HD2	1:D:172:GLY:O	2.13	0.47
1:A:65:GLY:O	1:A:69:THR:HG23	2.15	0.47
1:A:122:THR:HG23	1:A:125:ASP:H	1.79	0.47
1:A:434:THR:HA	1:A:437:LYS:HE2	1.96	0.47
1:C:208:ASN:HA	1:C:214:TYR:CE1	2.50	0.47
1:D:358:GLN:O	1:D:361:LEU:HB2	2.15	0.47
1:A:167:LEU:HB2	1:A:378:LEU:HD13	1.97	0.47
1:B:392:VAL:HG21	1:B:436:LEU:HD21	1.97	0.47
1:C:131:HIS:CD2	1:C:343:LEU:HD13	2.50	0.47
1:C:448:ALA:O	1:C:452:VAL:HG23	2.15	0.47
1:C:147:TRP:CH2	1:C:198:LEU:HD22	2.50	0.47
1:A:12:VAL:O	1:A:17:GLY:HA2	2.15	0.46
1:B:429:PRO:HG2	1:B:432:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:PRO:HD2	1:C:444:TYR:CD2	2.50	0.46
1:A:395:ARG:HG3	1:D:221:TYR:CZ	2.51	0.46
1:B:46:LYS:HG2	1:B:229:PHE:CE2	2.50	0.46
1:C:197:GLN:O	1:C:201:VAL:HG23	2.14	0.46
1:D:105:ALA:HA	1:D:111:HIS:HB2	1.96	0.46
1:B:163:ASP:O	1:B:165:PRO:HD3	2.16	0.46
1:D:221:TYR:HB3	1:D:224:VAL:HG23	1.97	0.46
1:A:324:LEU:HD22	1:A:342:VAL:CG1	2.45	0.46
1:D:217:HIS:HB3	1:D:226:TRP:CD2	2.50	0.46
1:A:38:GLN:O	1:A:42:ARG:HG2	2.16	0.46
1:B:37:VAL:HG13	1:B:100:LEU:HD21	1.96	0.46
1:A:176:THR:HA	1:A:177:PRO:HD3	1.81	0.46
1:C:385:LEU:C	1:C:388:PRO:HD2	2.35	0.46
1:A:89:THR:O	1:A:90:ASN:HB2	2.16	0.46
1:A:250:PRO:O	1:A:329:PRO:HA	2.15	0.46
1:B:206:LYS:C	1:B:206:LYS:HD2	2.36	0.46
1:C:107:ILE:HD12	1:C:107:ILE:N	2.31	0.46
1:A:55:GLU:HG2	1:D:395:ARG:O	2.16	0.46
1:B:198:LEU:HB2	1:B:260:CYS:SG	2.56	0.46
1:D:396:TYR:CE2	1:D:432:GLU:HG3	2.51	0.46
1:A:217:HIS:HB3	1:A:226:TRP:CD2	2.51	0.46
1:A:314:LEU:HG	1:A:356:ALA:HB1	1.96	0.46
1:A:388:PRO:HB3	1:A:444:TYR:CZ	2.50	0.46
1:B:125:ASP:CB	1:B:207:ILE:HG22	2.41	0.46
1:A:86:GLU:O	1:A:87:ARG:HB2	2.16	0.45
1:A:298:MET:HB3	1:A:299:PRO:HD2	1.98	0.45
1:B:250:PRO:O	1:B:251:HIS:HB2	2.16	0.45
1:C:204:LEU:HA	1:C:240:GLN:O	2.17	0.45
1:A:86:GLU:O	1:A:87:ARG:CB	2.63	0.45
1:A:131:HIS:CE1	1:A:343:LEU:HD13	2.52	0.45
1:B:167:LEU:HB2	1:B:378:LEU:HD12	1.97	0.45
1:A:203:ILE:O	1:A:240:GLN:HG3	2.16	0.45
1:B:11:PRO:HA	1:B:14:GLY:HA3	1.98	0.45
1:D:43:TRP:CZ3	1:D:207:ILE:HD13	2.52	0.45
1:D:362:LYS:O	1:D:366:LYS:HG3	2.16	0.45
1:B:167:LEU:HB2	1:B:378:LEU:CD1	2.47	0.45
1:C:27:PHE:CG	1:C:347:GLY:HA3	2.52	0.45
1:C:153:ALA:HB1	1:C:364:VAL:HG11	1.98	0.45
1:D:338:THR:O	1:D:342:VAL:HG23	2.16	0.45
1:A:447:ARG:O	1:A:447:ARG:HG2	2.16	0.45
1:B:173:GLN:HB3	1:B:174:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:GLU:OE2	1:C:433:LYS:HD2	2.17	0.45
1:D:430:GLU:O	1:D:434:THR:HG23	2.16	0.45
1:B:180:LEU:O	1:B:184:MET:HG2	2.17	0.45
1:D:42:ARG:HD3	1:D:45:GLN:OE1	2.16	0.45
1:B:429:PRO:HG2	1:B:432:GLU:CG	2.46	0.45
1:B:382:TRP:O	1:B:385:LEU:HB2	2.16	0.44
1:C:268:LEU:HD23	1:C:314:LEU:HD11	1.99	0.44
1:A:324:LEU:CD2	1:A:342:VAL:HG13	2.46	0.44
1:A:304:PRO:O	1:A:308:GLU:HG3	2.17	0.44
1:B:176:THR:HA	1:B:177:PRO:HD3	1.82	0.44
1:C:23:LEU:HD22	1:C:27:PHE:CE2	2.53	0.44
1:C:29:GLU:O	1:C:33:LEU:HG	2.18	0.44
1:D:279:ILE:HG12	1:D:284:PHE:HB2	1.99	0.44
1:A:250:PRO:O	1:A:251:HIS:HB2	2.17	0.44
1:D:354:LEU:O	1:D:358:GLN:HG3	2.17	0.44
1:A:6:LEU:O	1:B:28:SER:HB2	2.18	0.44
1:A:243:PRO:HG2	1:A:244:TYR:CD2	2.53	0.44
1:C:405:LEU:O	1:C:406:LYS:HB3	2.17	0.44
1:D:250:PRO:O	1:D:251:HIS:HB2	2.17	0.44
1:B:172:GLY:N	1:D:276:TRP:CZ2	2.85	0.44
1:D:197:GLN:O	1:D:201:VAL:HG23	2.18	0.44
1:A:147:TRP:CH2	1:A:198:LEU:HD22	2.53	0.44
1:A:171:HIS:O	1:A:173:GLN:HG3	2.18	0.44
1:B:197:GLN:HE22	1:C:256:GLU:CD	2.21	0.44
1:C:55:GLU:N	1:C:55:GLU:OE1	2.51	0.44
1:D:151:ILE:HG12	1:D:191:MET:HB3	1.99	0.44
1:D:259:ASP:O	1:D:263:ARG:HG3	2.18	0.44
1:A:55:GLU:HB3	1:A:116:PHE:CZ	2.53	0.43
1:C:11:PRO:HG3	1:D:345:ASN:ND2	2.32	0.43
1:D:46:LYS:HG2	1:D:229:PHE:CZ	2.53	0.43
1:B:111:HIS:HA	1:B:114:SER:HB3	2.00	0.43
1:D:390:GLN:HB2	1:D:405:LEU:HD13	1.99	0.43
1:A:115:GLU:O	1:D:394:ARG:HD3	2.17	0.43
1:B:23:LEU:HD11	1:B:354:LEU:HD22	1.98	0.43
1:B:89:THR:C	1:B:91:HIS:H	2.22	0.43
1:B:395:ARG:HG3	1:C:221:TYR:OH	2.19	0.43
1:A:157:LEU:HD11	1:A:364:VAL:HG13	1.99	0.43
1:B:335:ARG:HG2	1:B:336:ASP:H	1.83	0.43
1:B:388:PRO:O	1:B:392:VAL:HG23	2.19	0.43
1:C:151:ILE:HG12	1:C:191:MET:HB3	2.01	0.43
1:B:144:LEU:HB2	1:B:145:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ILE:H	1:B:207:ILE:HG13	1.59	0.43
1:C:400:LYS:O	1:C:404:LYS:HG2	2.18	0.43
1:A:243:PRO:HG2	1:A:244:TYR:HD2	1.83	0.43
1:A:305:ILE:HD13	1:A:308:GLU:OE1	2.19	0.43
1:A:50:HIS:CE1	1:A:224:VAL:HG13	2.53	0.43
1:B:320:VAL:HG11	1:B:348:VAL:HG23	1.99	0.43
1:C:201:VAL:HG11	1:C:257:LEU:HD23	2.00	0.43
1:D:247:GLN:HG2	1:D:335:ARG:HD2	2.00	0.43
1:C:383:GLU:HG3	1:C:414:VAL:CG2	2.48	0.43
1:B:193:ARG:O	1:B:197:GLN:HG3	2.19	0.43
1:D:272:ASP:OD1	1:D:307:PHE:HD1	2.01	0.43
1:A:335:ARG:HH21	1:A:337:LEU:HG	1.81	0.43
1:B:301:LYS:HB3	1:D:173:GLN:HE22	1.83	0.43
1:C:245:THR:HG22	1:C:246:THR:N	2.34	0.43
1:D:352:TYR:HA	1:D:355:ILE:HD12	2.01	0.43
1:A:11:PRO:HB2	1:A:16:TYR:CD2	2.54	0.42
1:B:243:PRO:HG2	1:B:244:TYR:CD2	2.54	0.42
1:B:384:VAL:HG23	1:B:385:LEU:HD23	2.01	0.42
1:A:158:ALA:HA	1:A:181:GLY:HA2	2.00	0.42
1:B:211:VAL:HG11	1:C:176:THR:O	2.18	0.42
1:C:324:LEU:HD22	1:C:342:VAL:HG13	2.00	0.42
1:D:207:ILE:HD11	1:D:230:SER:HA	2.01	0.42
1:A:213:ASN:HB2	1:A:215:ASN:HD21	1.83	0.42
1:A:104:VAL:HG13	1:A:110:LEU:HB2	2.00	0.42
1:C:328:LEU:HB2	1:C:329:PRO:HD3	2.01	0.42
1:D:147:TRP:O	1:D:151:ILE:HG13	2.19	0.42
1:A:211:VAL:HG22	1:D:176:THR:HB	2.01	0.42
1:B:392:VAL:O	1:B:396:TYR:HD2	2.03	0.42
1:D:162:ARG:HA	1:D:181:GLY:HA3	2.01	0.42
1:A:177:PRO:HB2	1:A:444:TYR:O	2.20	0.42
1:A:248:ILE:HG22	1:A:335:ARG:HH11	1.85	0.42
1:C:430:GLU:O	1:C:434:THR:HG23	2.20	0.42
1:D:208:ASN:CB	1:D:212:GLY:HA2	2.49	0.42
1:A:400:LYS:O	1:A:404:LYS:HG3	2.19	0.42
1:D:104:VAL:CG2	1:D:110:LEU:HD13	2.50	0.42
1:D:371:ARG:O	1:D:375:LEU:HG	2.20	0.42
1:A:104:VAL:HG12	1:A:104:VAL:O	2.20	0.42
1:A:348:VAL:HG12	1:A:352:TYR:CE2	2.55	0.42
1:B:206:LYS:HD2	1:B:206:LYS:O	2.20	0.42
1:C:193:ARG:O	1:C:197:GLN:HG3	2.19	0.42
1:C:217:HIS:HB3	1:C:226:TRP:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:HIS:HD2	1:D:173:GLN:HG3	1.85	0.42
1:A:371:ARG:O	1:A:375:LEU:HG	2.19	0.42
1:B:246:THR:HB	1:B:334:GLN:O	2.19	0.42
1:A:252:ASP:O	1:A:255:ALA:HB3	2.20	0.42
1:A:265:ASN:O	1:A:269:ILE:HG13	2.20	0.42
1:B:41:VAL:O	1:B:45:GLN:HG3	2.20	0.42
1:D:100:LEU:O	1:D:104:VAL:HB	2.19	0.42
1:D:154:VAL:HG11	1:D:187:VAL:HB	2.01	0.42
1:D:213:ASN:HB2	1:D:215:ASN:OD1	2.20	0.42
1:A:26:ILE:O	1:A:31:GLY:HA3	2.20	0.41
1:A:218:ILE:HD11	1:D:447:ARG:HB2	2.02	0.41
1:A:257:LEU:O	1:A:261:ILE:HG13	2.20	0.41
1:A:284:PHE:HD1	1:A:368:GLU:O	2.03	0.41
1:A:316:LEU:O	1:A:319:ALA:HB3	2.20	0.41
1:D:354:LEU:HD12	1:D:354:LEU:HA	1.87	0.41
1:A:447:ARG:HH11	1:A:451:LEU:HG	1.85	0.41
1:C:170:THR:O	1:C:171:HIS:CG	2.73	0.41
1:D:189:TYR:O	1:D:193:ARG:HG3	2.21	0.41
1:D:81:ARG:O	1:D:85:ILE:HG13	2.19	0.41
1:B:107:ILE:HA	1:B:108:PRO:HD3	1.93	0.41
1:B:333:TRP:HB3	1:B:334:GLN:H	1.61	0.41
1:C:162:ARG:HD2	1:C:449:VAL:HG13	2.02	0.41
1:D:271:PHE:O	1:D:275:VAL:HG23	2.20	0.41
1:C:12:VAL:O	1:C:17:GLY:HA2	2.21	0.41
1:C:32:LEU:HD21	1:C:36:ARG:NH2	2.36	0.41
1:C:324:LEU:HD22	1:C:342:VAL:CG1	2.50	0.41
1:D:183:GLU:O	1:D:187:VAL:HG23	2.21	0.41
1:D:355:ILE:O	1:D:359:SER:HB2	2.20	0.41
1:D:447:ARG:HG2	1:D:447:ARG:O	2.20	0.41
1:A:122:THR:O	1:A:125:ASP:HB2	2.21	0.41
1:B:179:THR:CG2	1:B:445:ILE:HG21	2.39	0.41
1:A:285:LYS:HD2	1:A:299:PRO:HB3	2.02	0.41
1:A:339:ASP:HA	1:A:342:VAL:HB	2.02	0.41
1:B:328:LEU:HB2	1:B:329:PRO:HD3	2.03	0.41
1:D:20:VAL:CG1	1:D:23:LEU:HD12	2.50	0.41
1:A:108:PRO:HA	1:A:111:HIS:HB3	2.02	0.41
1:B:34:LYS:NZ	3:B:608:HOH:O	2.52	0.41
1:D:107:ILE:N	1:D:107:ILE:HD12	2.35	0.41
1:D:279:ILE:HD12	1:D:304:PRO:HB3	2.02	0.41
1:A:447:ARG:HB2	1:D:218:ILE:CD1	2.50	0.41
1:B:169:ARG:HA	1:B:173:GLN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:THR:O	1:B:171:HIS:CG	2.73	0.41
1:B:338:THR:O	1:B:342:VAL:HG23	2.20	0.41
1:C:353:ALA:HB1	1:C:357:TYR:CZ	2.56	0.41
1:A:314:LEU:HG	1:A:356:ALA:CB	2.51	0.41
1:B:423:ILE:HD13	1:B:436:LEU:HB3	2.02	0.41
1:C:258:PHE:CD1	1:C:321:LEU:HD22	2.56	0.41
1:A:396:TYR:CE1	1:A:429:PRO:HG2	2.57	0.40
1:C:228:GLN:O	1:C:232:GLU:HG3	2.22	0.40
1:D:107:ILE:HA	1:D:108:PRO:HD3	1.82	0.40
1:A:324:LEU:HB3	1:A:328:LEU:HD12	2.03	0.40
1:A:394:ARG:HD3	1:D:115:GLU:O	2.20	0.40
1:C:42:ARG:HH12	1:C:45:GLN:HE22	1.70	0.40
1:C:46:LYS:HD3	1:C:233:PHE:HB2	2.03	0.40
1:C:190:ARG:HB3	1:C:267:ILE:HD13	2.04	0.40
1:A:34:LYS:HG3	1:A:74:PHE:CD2	2.57	0.40
1:A:166:LEU:N	1:A:178:SER:O	2.46	0.40
1:A:307:PHE:O	1:A:310:SER:HB3	2.22	0.40
1:A:328:LEU:HB2	1:A:329:PRO:HD3	2.02	0.40
1:B:131:HIS:CE1	1:B:343:LEU:HD13	2.56	0.40
1:A:104:VAL:HG11	1:A:110:LEU:HB3	2.03	0.40
1:A:128:ASN:HD21	1:A:129:LEU:HD13	1.87	0.40
1:A:334:GLN:O	1:A:335:ARG:CB	2.68	0.40
1:B:257:LEU:O	1:B:261:ILE:HG13	2.21	0.40
1:A:445:ILE:H	1:A:445:ILE:HG13	1.61	0.40
1:D:150:VAL:O	1:D:154:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	440/470 (94%)	419 (95%)	21 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	441/470 (94%)	420 (95%)	21 (5%)	0	100	100
1	C	442/470 (94%)	425 (96%)	16 (4%)	1 (0%)	47	82
1	D	437/470 (93%)	423 (97%)	13 (3%)	1 (0%)	47	82
All	All	1760/1880 (94%)	1687 (96%)	71 (4%)	2 (0%)	51	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	210	ALA
1	D	210	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/399 (92%)	342 (93%)	25 (7%)	16	48
1	B	358/399 (90%)	334 (93%)	24 (7%)	16	49
1	C	364/399 (91%)	333 (92%)	31 (8%)	10	38
1	D	361/399 (90%)	336 (93%)	25 (7%)	15	48
All	All	1450/1596 (91%)	1345 (93%)	105 (7%)	14	45

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	SER
1	A	62	ASP
1	A	76	GLU
1	A	91	HIS
1	A	128	ASN
1	A	171	HIS
1	A	196	ARG
1	A	197	GLN

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Mol	Chain	Res	Type
1	A	204	LEU
1	A	208	ASN
1	A	235	THR
1	A	301	LYS
1	A	306	ASP
1	A	335	ARG
1	A	339	ASP
1	A	341	THR
1	A	354	LEU
1	A	359	SER
1	A	365	SER
1	A	376	ASP
1	A	378	LEU
1	A	434	THR
1	A	440	THR
1	A	445	ILE
1	B	1	MET
1	B	7	THR
1	B	15	ARG
1	B	32	LEU
1	B	62	ASP
1	B	64	ASN
1	B	67	LEU
1	B	88	THR
1	B	128	ASN
1	B	207	ILE
1	B	227	HIS
1	B	254	ILE
1	B	257	LEU
1	B	287	LYS
1	B	327	LYS
1	B	331	SER
1	B	377	GLU
1	B	380	HIS
1	B	385	LEU
1	B	391	THR
1	B	409	THR
1	B	415	ASP
1	B	419	MET
1	B	445	ILE
1	C	15	ARG
1	C	84	THR

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Mol	Chain	Res	Type
1	C	104	VAL
1	C	114	SER
1	C	128	ASN
1	C	159	THR
1	C	166	LEU
1	C	182	LYS
1	C	208	ASN
1	C	217	HIS
1	C	223	GLU
1	C	227	HIS
1	C	228	GLN
1	C	288	THR
1	C	301	LYS
1	C	302	VAL
1	C	303	ASN
1	C	331	SER
1	C	348	VAL
1	C	359	SER
1	C	380	HIS
1	C	394	ARG
1	C	395	ARG
1	C	405	LEU
1	C	407	GLU
1	C	408	LEU
1	C	423	ILE
1	C	425	SER
1	C	440	THR
1	C	447	ARG
1	C	450	THR
1	D	1	MET
1	D	4	SER
1	D	10	SER
1	D	21	SER
1	D	56	VAL
1	D	62	ASP
1	D	76	GLU
1	D	104	VAL
1	D	114	SER
1	D	122	THR
1	D	128	ASN
1	D	160	GLN
1	D	162	ARG

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Mol	Chain	Res	Type
1	D	166	LEU
1	D	207	ILE
1	D	227	HIS
1	D	306	ASP
1	D	327	LYS
1	D	331	SER
1	D	354	LEU
1	D	359	SER
1	D	391	THR
1	D	415	ASP
1	D	425	SER
1	D	449	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	HIS
1	A	215	ASN
1	A	373	HIS
1	B	91	HIS
1	B	265	ASN
1	B	283	HIS
1	C	381	ASN
1	D	131	HIS
1	D	171	HIS
1	D	208	ASN
1	D	322	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	N2P	C	501	-	6,6,6	0.41	0	5,5,5	0.55	0
2	N2P	B	501	-	6,6,6	0.18	0	5,5,5	0.55	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
2	N2P	C	501	-	-	0/4/4/4	-
2	N2P	B	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	446/470 (94%)	-0.31	6 (1%)	77	51	20, 34, 53, 71	0
1	B	447/470 (95%)	-0.24	6 (1%)	77	51	22, 31, 58, 70	0
1	C	446/470 (94%)	-0.28	3 (0%)	87	69	22, 32, 53, 74	0
1	D	443/470 (94%)	-0.25	3 (0%)	87	69	22, 32, 60, 70	0
All	All	1782/1880 (94%)	-0.27	18 (1%)	82	59	20, 32, 56, 74	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	409	THR	3.6
1	C	411	GLY	3.1
1	B	289	ILE	2.7
1	B	421	GLN	2.7
1	B	424	ASP	2.6
1	A	288	THR	2.6
1	D	405	LEU	2.5
1	A	406	LYS	2.5
1	B	431	ALA	2.4
1	C	412	LYS	2.4
1	A	90	ASN	2.4
1	D	299	PRO	2.3
1	A	434	THR	2.2
1	A	298	MET	2.2
1	D	406	LYS	2.1
1	B	425	SER	2.1
1	B	417	GLU	2.1
1	A	98	TYR	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	N2P	B	501	7/7	0.87	0.39	21,22,27,29	0
2	N2P	C	501	7/7	0.88	0.39	18,26,29,30	0

6.5 Other polymers (i)

There are no such residues in this entry.