Full wwPDB X-ray Structure Validation Report (i)

Nov 4, 2023 – 08:47 PM EDT

PDB ID	:	2GVQ
Title	:	Anthranilate phosphoribosyl-transferase (TRPD) from S. solfataricus in complex with anthranilate
Authors	:	Marino, M.; Deuss, M.; Sterner, R.; Mayans, O.
Deposited on	:	2006-05-03
Resolution	:	2.43 Å(reported)

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

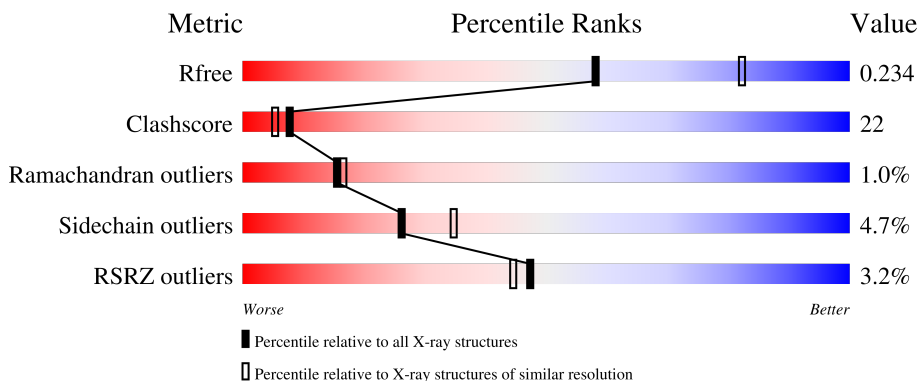|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.43 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.234
Clashscore		22
Ramachandran outliers		1.0%
Sidechain outliers		4.7%
RSRZ outliers		3.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	345	2% — 63% / 32%
1	B	345	3% — 60% / 36%
1	C	345	4% — 63% / 33%
1	D	345	3% — 61% / 36%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10826 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 Anthranilate phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2618	1679	441	491	7			
1	B	340	Total	C	N	O	S	0	0	0
			2618	1679	441	491	7			
1	C	341	Total	C	N	O	S	0	0	0
			2622	1680	442	493	7			
1	D	345	Total	C	N	O	S	0	0	0
			2645	1692	446	500	7			

- Molecule 2 is 2-AMINOBENZOIC ACID (three-letter code: BE2) (formula: $C_7H_7NO_2$).
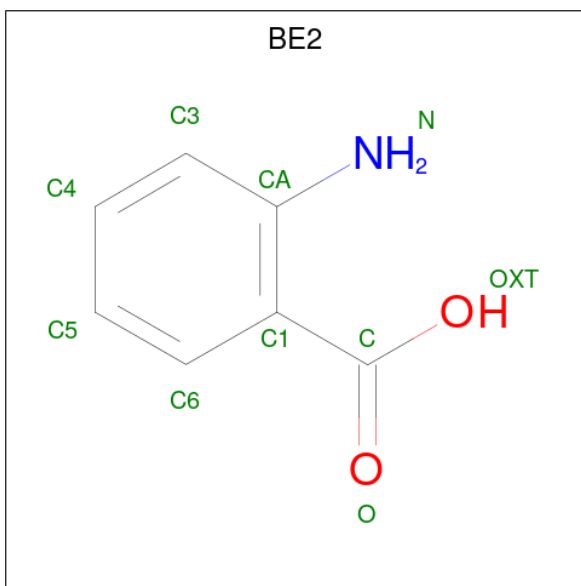
BE2

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	7	1	2		
2	B	1	Total	C	N	O	0	0
			10	7	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 10	C 7	N 1	O 2	0	0
2	C	1	Total 10	C 7	N 1	O 2	0	0
2	C	1	Total 10	C 7	N 1	O 2	0	0
2	D	1	Total 10	C 7	N 1	O 2	0	0
2	D	1	Total 10	C 7	N 1	O 2	0	0

• Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total 83	O 83	0	0
3	B	53	Total 53	O 53	0	0
3	C	60	Total 60	O 60	0	0
3	D	57	Total 57	O 57	0	0

3 Residue-property plots ⓘ

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.

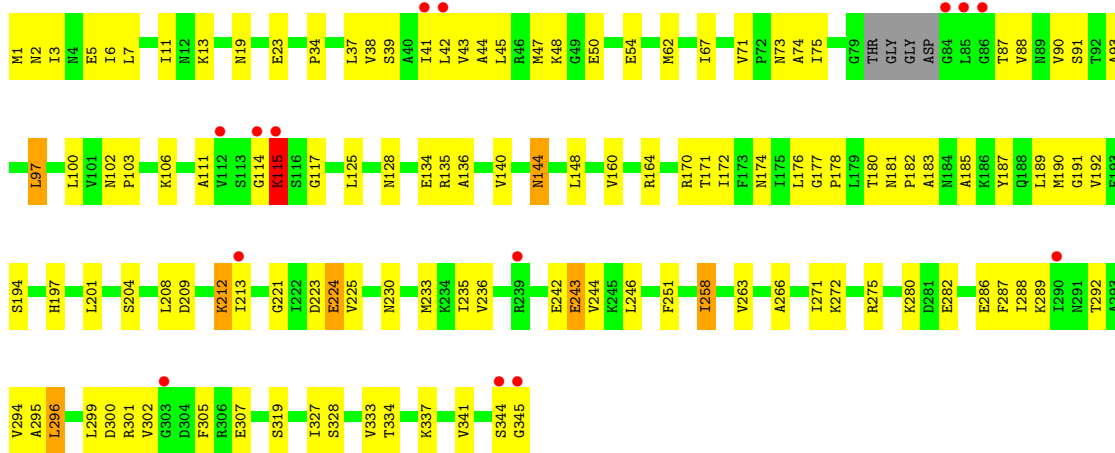- Molecule 1: Anthranilate phosphoribosyltransferase

Chain A:

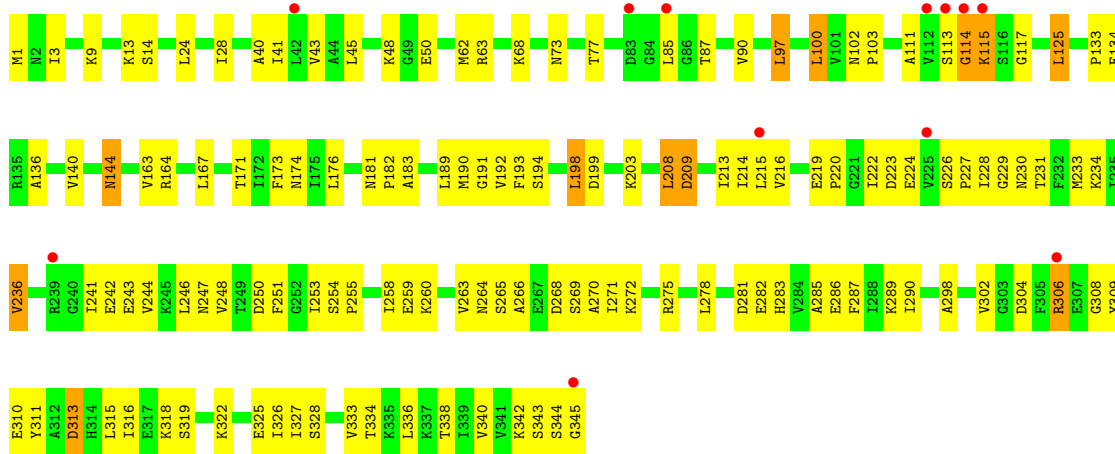- Molecule 1: Anthranilate phosphoribosyltransferase

Chain B:

- Molecule 1: Anthranilate phosphoribosyltransferase

Chain C:

• Molecule 1: Anthranilate phosphoribosyltransferase

Chain D:
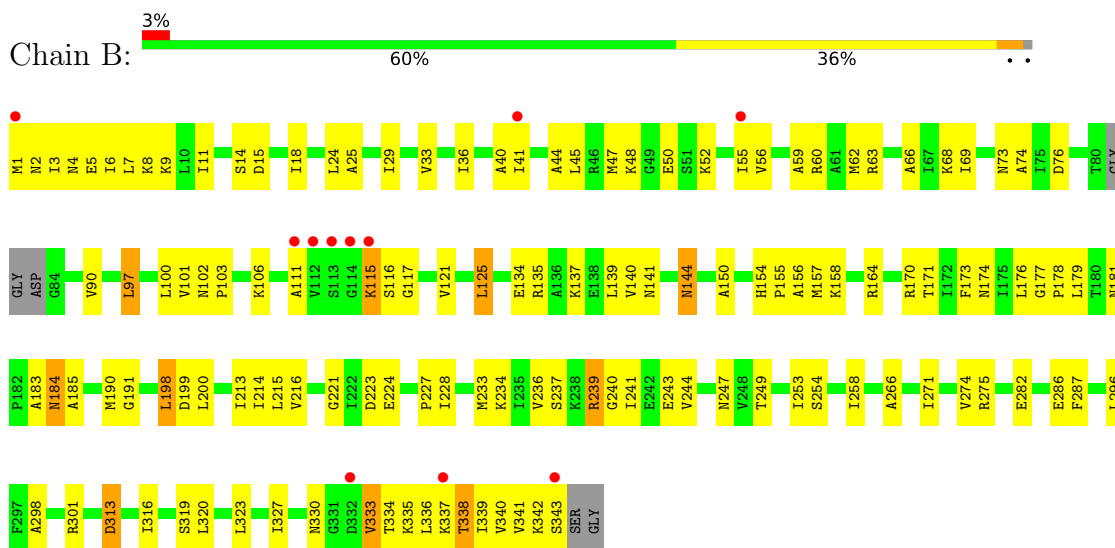
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	91.81Å 65.62Å 115.61Å 90.00° 107.39° 90.00°	Depositor
Resolution (Å)	20.00 – 2.43 19.34 – 2.43	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.43) 99.3 (19.34-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.43Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.242 0.192 , 0.234	Depositor DCC
R_{free} test set	584 reflections (1.18%)	wwPDB-VP
Wilson B-factor (Å^2)	54.9	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.6	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10826	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: BE2

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	0/2654	0.65	0/3585
1	B	0.38	0/2654	0.64	1/3585 (0.0%)
1	C	0.37	0/2658	0.62	0/3588
1	D	0.37	0/2682	0.63	0/3622
All	All	0.38	0/10648	0.64	1/14380 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	97	LEU	CA-CB-CG	6.20	129.56	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	TYR	Sidechain

WORLDWIDE

wwPDB

PROTEIN DATA BANK

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	2618	0	2737	103	0
1	B	2618	0	2737	148	0
1	C	2622	0	2738	100	1
1	D	2645	0	2756	131	0
2	A	10	0	3	0	0
2	B	20	0	6	0	0
2	C	20	0	6	1	0
2	D	20	0	6	1	0
3	A	83	0	0	7	0
3	B	53	0	0	5	0
3	C	60	0	0	3	0
3	D	57	0	0	1	0
All	All	10826	0	10989	471	1

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 (471) 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:62:MET:HE1	1:C:176:LEU:HD13	1.32	1.10
1:D:62:MET:HE1	1:D:176:LEU:HD13	1.33	1.06
1:D:85:LEU:HD12	1:D:85:LEU:H	1.24	1.02
1:D:263:VAL:HG13	1:D:268:ASP:HB2	1.37	1.02
1:A:115:LYS:HB3	1:A:266:ALA:HB2	1.44	0.98
1:A:171:THR:H	1:A:174:ASN:HD22	1.12	0.96
1:C:171:THR:H	1:C:174:ASN:HD22	1.14	0.94
1:D:171:THR:H	1:D:174:ASN:HD22	1.16	0.92
1:C:115:LYS:HB3	1:C:266:ALA:HB2	1.51	0.92
1:B:171:THR:H	1:B:174:ASN:ND2	1.71	0.89
1:A:171:THR:H	1:A:174:ASN:ND2	1.70	0.88
1:B:2:ASN:HB3	1:B:5:GLU:HG3	1.56	0.86
1:B:236:VAL:HG22	1:B:241:ILE:HG12	1.56	0.86
1:B:216:VAL:HG12	1:B:233:MET:HB3	1.57	0.84
1:A:97:LEU:HD22	1:A:319:SER:OG	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:THR:H	1:B:174:ASN:HD22	1.25	0.84
1:B:253:ILE:HG22	1:B:254:SER:H	1.43	0.84
1:B:102:ASN:HD22	1:B:301:ARG:NH2	1.76	0.83
1:B:97:LEU:HD22	1:B:319:SER:OG	1.79	0.82
1:B:271:ILE:HG23	1:B:342:LYS:HG3	1.60	0.82
1:B:339:ILE:HA	1:B:342:LYS:HD3	1.61	0.81
1:C:62:MET:HE3	1:C:176:LEU:HB3	1.61	0.81
1:A:342:LYS:HE2	1:A:342:LYS:HA	1.63	0.81
1:A:115:LYS:CB	1:A:266:ALA:HB2	2.11	0.80
1:B:29:ILE:HG22	1:B:156:ALA:HB1	1.63	0.80
1:A:282:GLU:O	1:A:286:GLU:HG2	1.81	0.80
1:C:97:LEU:HD22	1:C:319:SER:OG	1.81	0.80
1:B:338:THR:HB	1:B:342:LYS:HZ2	1.46	0.80
1:D:220:PRO:HD3	1:D:226:SER:OG	1.83	0.79
1:B:271:ILE:HA	1:B:342:LYS:HE2	1.63	0.79
1:B:275:ARG:HG2	1:B:342:LYS:HB3	1.65	0.77
1:A:102:ASN:HD22	1:A:301:ARG:NH2	1.82	0.77
1:C:171:THR:H	1:C:174:ASN:ND2	1.86	0.74
1:A:3:ILE:HD12	1:A:37:LEU:HD13	1.69	0.74
1:A:115:LYS:HE2	1:A:115:LYS:H	1.51	0.74
1:B:253:ILE:HG22	1:B:254:SER:N	2.02	0.73
1:D:219:GLU:HB2	1:D:230:ASN:O	1.87	0.73
1:D:213:ILE:HG23	1:D:236:VAL:HG13	1.71	0.72
1:A:235:ILE:HB	1:A:242:GLU:HB2	1.72	0.72
1:B:247:ASN:HD22	1:B:249:THR:HB	1.55	0.71
1:B:274:VAL:HB	1:B:342:LYS:HE2	1.71	0.71
1:D:115:LYS:HB3	1:D:266:ALA:HB2	1.72	0.71
1:B:115:LYS:HB3	1:B:266:ALA:HB2	1.71	0.71
1:B:237:SER:OG	1:B:239:ARG:NE	2.23	0.71
1:B:3:ILE:HD11	1:B:41:ILE:HD11	1.73	0.70
1:B:271:ILE:HA	1:B:342:LYS:CE	2.20	0.70
1:B:336:LEU:HA	1:B:339:ILE:HG22	1.71	0.70
1:B:271:ILE:O	1:B:275:ARG:HG3	1.92	0.70
1:C:13:LYS:HA	1:C:48:LYS:HG3	1.73	0.69
1:D:85:LEU:H	1:D:85:LEU:CD1	2.02	0.69
1:B:338:THR:O	1:B:342:LYS:HD2	1.93	0.69
1:A:6:ILE:HG21	1:A:24:LEU:HD22	1.73	0.68
1:B:338:THR:HB	1:B:342:LYS:NZ	2.08	0.68
1:D:334:THR:O	1:D:338:THR:HG23	1.92	0.68
1:B:338:THR:CB	1:B:342:LYS:HZ2	2.06	0.68
1:A:160:VAL:HG12	1:A:160:VAL:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:GLU:O	1:D:286:GLU:HG3	1.94	0.67
1:A:327:ILE:HD12	1:A:336:LEU:HD22	1.77	0.67
1:B:171:THR:N	1:B:174:ASN:HD22	1.92	0.67
1:B:233:MET:HG3	1:B:244:VAL:HB	1.76	0.67
1:B:116:SER:HB2	3:B:410:HOH:O	1.94	0.67
1:B:178:PRO:HB2	1:B:190:MET:CE	2.25	0.67
1:B:336:LEU:HA	1:B:339:ILE:CG2	2.25	0.66
1:B:178:PRO:HB2	1:B:190:MET:HE2	1.77	0.66
1:D:171:THR:H	1:D:174:ASN:ND2	1.93	0.66
1:C:2:ASN:OD1	1:C:5:GLU:HB2	1.95	0.66
1:A:311:TYR:HE1	1:A:315:LEU:HD21	1.61	0.66
1:A:304:ASP:OD2	1:A:306:ARG:HB2	1.96	0.65
1:D:97:LEU:HD22	1:D:319:SER:OG	1.96	0.65
1:D:219:GLU:OE1	1:D:229:GLY:HA3	1.97	0.65
1:D:336:LEU:O	1:D:340:VAL:HG23	1.97	0.65
1:C:189:LEU:HD12	1:C:295:ALA:HB2	1.79	0.65
1:A:63:ARG:O	1:A:68:LYS:HE2	1.97	0.65
1:D:125:LEU:O	1:D:327:ILE:HD13	1.97	0.65
1:C:62:MET:CE	1:C:176:LEU:HB3	2.25	0.65
1:D:220:PRO:HG3	1:D:228:ILE:CD1	2.27	0.65
1:A:24:LEU:HD11	1:A:41:ILE:HD13	1.79	0.64
1:A:282:GLU:HG3	3:A:423:HOH:O	1.98	0.64
1:D:327:ILE:HD12	1:D:336:LEU:HD22	1.79	0.64
1:A:29:ILE:HG22	1:A:156:ALA:HB1	1.79	0.64
1:A:62:MET:CE	1:A:176:LEU:HB3	2.28	0.64
1:D:253:ILE:HG22	1:D:254:SER:N	2.13	0.64
1:D:263:VAL:CG1	1:D:268:ASP:HB2	2.20	0.63
1:D:228:ILE:HG13	1:D:229:GLY:N	2.13	0.63
1:A:213:ILE:HG23	1:A:236:VAL:HB	1.80	0.63
1:A:285:ALA:O	1:A:289:LYS:HG3	1.99	0.63
1:B:184:ASN:CG	1:B:184:ASN:O	2.36	0.63
1:D:62:MET:CE	1:D:176:LEU:HD13	2.19	0.63
1:D:164:ARG:NH2	2:D:602:BE2:N	2.46	0.63
1:A:170:ARG:NH1	1:A:193:PHE:HE2	1.96	0.63
1:B:24:LEU:HD11	1:B:41:ILE:HD13	1.81	0.63
1:B:40:ALA:HB1	1:C:43:VAL:HG21	1.81	0.62
1:C:1:MET:CE	1:C:6:ILE:HD11	2.29	0.62
1:A:164:ARG:HD2	3:A:362:HOH:O	1.98	0.62
1:B:191:GLY:HA3	1:B:223:ASP:O	1.99	0.62
1:D:13:LYS:HA	1:D:48:LYS:HG3	1.81	0.62
1:B:170:ARG:NH1	3:B:424:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:PRO:HG3	1:D:228:ILE:HG12	1.81	0.61
1:A:136:ALA:O	1:A:140:VAL:HG23	1.99	0.61
1:A:171:THR:N	1:A:174:ASN:HD22	1.92	0.61
1:C:62:MET:HE1	1:C:176:LEU:CD1	2.20	0.61
1:C:302:VAL:HG13	1:C:307:GLU:CD	2.20	0.60
1:A:160:VAL:HG12	1:A:164:ARG:HG3	1.83	0.60
1:B:274:VAL:HG21	1:B:342:LYS:NZ	2.16	0.60
1:A:135:ARG:HG3	1:A:135:ARG:HH11	1.65	0.60
1:C:280:LYS:HE3	1:C:345:GLY:N	2.17	0.60
1:D:73:ASN:HD22	1:D:103:PRO:HG3	1.67	0.60
1:D:289:LYS:HE2	1:D:313:ASP:HA	1.84	0.60
1:A:336:LEU:O	1:A:340:VAL:HG23	2.02	0.60
1:B:323:LEU:HD23	1:B:335:LYS:HE3	1.82	0.60
1:D:97:LEU:O	1:D:100:LEU:HB2	2.03	0.59
1:A:90:VAL:HG11	1:A:287:PHE:CD2	2.37	0.59
1:C:48:LYS:NZ	1:C:54:GLU:OE2	2.36	0.59
1:D:87:THR:HG21	1:D:224:GLU:OE1	2.01	0.59
1:B:334:THR:HG22	1:B:334:THR:O	2.03	0.59
1:B:338:THR:C	1:B:342:LYS:HZ2	2.05	0.59
1:D:199:ASP:OD1	1:D:203:LYS:HE3	2.02	0.59
1:A:62:MET:HE1	1:A:176:LEU:CB	2.33	0.59
1:C:164:ARG:NH2	2:C:502:BE2:N	2.49	0.59
1:D:259:GLU:CD	1:D:259:GLU:H	2.06	0.59
1:D:340:VAL:HG12	1:D:345:GLY:HA3	1.84	0.59
1:C:115:LYS:NZ	3:C:523:HOH:O	2.35	0.58
1:A:62:MET:CE	1:A:180:THR:HG21	2.33	0.58
1:B:336:LEU:CA	1:B:339:ILE:HG22	2.32	0.58
1:B:274:VAL:HB	1:B:342:LYS:CE	2.33	0.58
1:A:337:LYS:O	1:A:341:VAL:HG23	2.04	0.58
1:B:343:SER:HA	3:B:426:HOH:O	2.01	0.58
1:B:253:ILE:CG2	1:B:254:SER:H	2.16	0.58
1:C:171:THR:N	1:C:174:ASN:HD22	1.95	0.58
1:A:13:LYS:HA	1:A:48:LYS:HG3	1.85	0.58
1:D:260:LYS:N	1:D:260:LYS:HD2	2.18	0.58
1:B:275:ARG:HG2	1:B:342:LYS:CB	2.34	0.58
1:D:125:LEU:HB3	1:D:327:ILE:HD11	1.85	0.58
1:D:24:LEU:O	1:D:28:ILE:HG13	2.03	0.58
1:C:194:SER:OG	1:C:197:HIS:HD2	1.87	0.57
1:D:62:MET:HE1	1:D:176:LEU:CD1	2.21	0.57
1:D:63:ARG:O	1:D:68:LYS:HE3	2.04	0.57
1:D:253:ILE:HD11	1:D:309:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:MET:HE3	1:A:180:THR:HG21	1.84	0.57
1:C:134:GLU:HG2	1:C:135:ARG:N	2.20	0.57
1:B:73:ASN:ND2	1:B:103:PRO:HG3	2.19	0.57
1:C:19:ASN:O	1:C:23:GLU:HG2	2.05	0.57
1:D:338:THR:O	1:D:342:LYS:HG3	2.04	0.57
1:B:213:ILE:HG23	1:B:236:VAL:HB	1.86	0.57
1:A:115:LYS:H	1:A:115:LYS:CE	2.18	0.57
1:B:338:THR:HG22	1:B:342:LYS:HE3	1.86	0.57
1:B:337:LYS:O	1:B:341:VAL:HG23	2.05	0.57
1:B:253:ILE:N	1:B:253:ILE:HD12	2.20	0.57
1:D:208:LEU:O	1:D:209:ASP:HB3	2.05	0.57
1:A:15:ASP:HA	1:A:48:LYS:NZ	2.20	0.57
1:D:192:VAL:HG12	1:D:194:SER:H	1.69	0.57
1:D:275:ARG:HG2	1:D:281:ASP:HB2	1.87	0.56
1:A:62:MET:HE1	1:A:176:LEU:HB3	1.86	0.56
1:A:115:LYS:HE2	1:A:115:LYS:N	2.20	0.56
1:A:335:LYS:O	1:A:339:ILE:HG12	2.05	0.56
1:B:2:ASN:HB3	1:B:5:GLU:CG	2.34	0.56
1:B:237:SER:OG	1:B:239:ARG:CD	2.53	0.56
1:B:170:ARG:HA	1:B:174:ASN:ND2	2.21	0.56
1:D:253:ILE:HD11	1:D:309:TYR:CZ	2.41	0.56
1:D:260:LYS:HG2	1:D:283:HIS:HD2	1.69	0.56
1:A:227:PRO:HB3	1:A:287:PHE:CD1	2.41	0.56
1:C:328:SER:HA	1:C:333:VAL:HG22	1.86	0.56
1:B:323:LEU:HB3	1:B:335:LYS:HZ1	1.69	0.56
1:C:128:ASN:HA	3:C:509:HOH:O	2.04	0.56
1:D:198:LEU:HD22	1:D:234:LYS:HG2	1.86	0.56
1:B:3:ILE:HD11	1:B:41:ILE:CD1	2.35	0.55
1:D:325:GLU:HG3	1:D:326:ILE:N	2.21	0.55
1:D:133:PRO:HG2	1:D:134:GLU:OE1	2.06	0.55
1:A:37:LEU:O	1:A:41:ILE:HG13	2.07	0.55
1:C:90:VAL:HG11	1:C:287:PHE:CD2	2.41	0.55
1:A:9:LYS:HE2	1:A:15:ASP:O	2.07	0.55
1:B:25:ALA:O	1:B:29:ILE:HG13	2.07	0.55
1:C:1:MET:HE2	1:C:6:ILE:HD11	1.87	0.55
1:C:136:ALA:O	1:C:140:VAL:HG23	2.07	0.55
1:C:233:MET:HG3	1:C:244:VAL:HB	1.89	0.55
1:D:163:VAL:HG23	3:D:611:HOH:O	2.06	0.55
1:C:235:ILE:HB	1:C:242:GLU:HB3	1.89	0.55
1:B:115:LYS:HD2	1:B:115:LYS:N	2.22	0.54
1:A:256:ILE:HD12	1:A:256:ILE:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ILE:O	1:B:183:ALA:HA	2.07	0.54
1:A:204:SER:O	1:A:208:LEU:HD22	2.07	0.54
1:D:271:ILE:HG23	1:D:343:SER:HB2	1.89	0.54
1:A:292:THR:HG22	1:A:296:LEU:HD22	1.90	0.54
1:C:271:ILE:O	1:C:275:ARG:HG3	2.06	0.54
1:B:339:ILE:HA	1:B:342:LYS:CD	2.33	0.54
1:B:247:ASN:HD22	1:B:249:THR:H	1.54	0.54
1:A:190:MET:O	1:A:190:MET:HG3	2.06	0.54
1:B:41:ILE:O	1:B:45:LEU:HB2	2.08	0.54
1:B:102:ASN:HD22	1:B:301:ARG:HH22	1.52	0.54
1:B:170:ARG:NH1	1:B:174:ASN:HB3	2.22	0.54
1:A:170:ARG:HH11	1:A:193:PHE:HE2	1.54	0.54
1:C:243:GLU:CD	1:C:243:GLU:H	2.11	0.54
1:D:102:ASN:CG	1:D:103:PRO:HD2	2.29	0.54
1:B:125:LEU:O	1:B:327:ILE:HD13	2.08	0.53
1:C:134:GLU:HG2	1:C:135:ARG:H	1.74	0.53
1:C:75:ILE:HG13	1:C:187:TYR:O	2.07	0.53
1:C:243:GLU:CD	1:C:243:GLU:N	2.61	0.53
1:A:115:LYS:HB3	1:A:120:ASP:HB3	1.91	0.53
1:A:275:ARG:HG2	1:A:343:SER:O	2.07	0.53
1:B:333:VAL:HG12	1:B:333:VAL:O	2.08	0.53
1:B:4:ASN:O	1:B:8:LYS:HG3	2.08	0.53
1:D:302:VAL:HG11	1:D:308:GLY:N	2.22	0.53
1:B:62:MET:CE	1:B:176:LEU:HD13	2.38	0.53
1:B:336:LEU:O	1:B:340:VAL:HG23	2.09	0.52
1:A:100:LEU:HD13	1:A:322:LYS:HG2	1.92	0.52
1:C:93:ALA:HB1	1:C:288:ILE:HD13	1.91	0.52
1:D:227:PRO:HG3	1:D:287:PHE:CE1	2.44	0.52
1:B:150:ALA:O	1:B:154:HIS:HB2	2.09	0.52
1:B:68:LYS:HE3	3:B:453:HOH:O	2.08	0.52
1:B:282:GLU:O	1:B:286:GLU:HG3	2.10	0.52
1:C:7:LEU:O	1:C:11:ILE:HG12	2.09	0.52
1:D:190:MET:O	1:D:215:LEU:HA	2.10	0.52
1:D:223:ASP:C	1:D:224:GLU:HG3	2.29	0.52
1:B:7:LEU:O	1:B:11:ILE:HG12	2.10	0.51
1:B:62:MET:HE3	1:B:176:LEU:HB3	1.92	0.51
1:B:198:LEU:HD22	1:B:234:LYS:CG	2.40	0.51
1:D:306:ARG:HG3	1:D:306:ARG:HH11	1.75	0.51
1:A:73:ASN:ND2	1:A:103:PRO:HG3	2.25	0.51
1:B:117:GLY:O	1:B:121:VAL:HG23	2.10	0.51
1:D:125:LEU:HD13	1:D:270:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:PRO:HG3	1:D:228:ILE:CG1	2.40	0.51
1:B:36:ILE:HG23	1:C:39:SER:HB2	1.92	0.51
1:D:282:GLU:HG3	1:D:283:HIS:H	1.74	0.51
1:A:73:ASN:HD22	1:A:103:PRO:HG3	1.76	0.51
1:B:198:LEU:HD22	1:B:234:LYS:HG2	1.91	0.51
1:C:328:SER:HA	1:C:333:VAL:CG2	2.40	0.51
1:D:198:LEU:HD22	1:D:234:LYS:CG	2.41	0.51
1:B:320:LEU:HD12	1:B:335:LYS:NZ	2.26	0.51
1:A:284:VAL:O	1:A:288:ILE:HG13	2.11	0.51
1:D:222:ILE:HG22	1:D:224:GLU:N	2.26	0.50
1:B:18:ILE:HG21	1:B:60:ARG:NH1	2.27	0.50
1:C:48:LYS:HZ1	1:C:54:GLU:CD	2.13	0.50
1:C:73:ASN:HD22	1:C:103:PRO:HG3	1.75	0.50
1:D:136:ALA:O	1:D:140:VAL:HG23	2.11	0.50
1:D:226:SER:O	1:D:248:VAL:HG22	2.11	0.50
1:D:287:PHE:O	1:D:290:ILE:HG12	2.11	0.50
1:B:135:ARG:HG3	1:B:135:ARG:HH11	1.76	0.50
1:B:274:VAL:HG21	1:B:342:LYS:HZ3	1.75	0.50
1:C:181:ASN:HD21	1:C:183:ALA:HB3	1.77	0.50
1:B:170:ARG:HH12	1:B:174:ASN:HB3	1.77	0.50
1:B:50:GLU:H	1:B:50:GLU:CD	2.15	0.50
1:D:73:ASN:ND2	1:D:103:PRO:HG3	2.27	0.50
1:A:15:ASP:HA	1:A:48:LYS:HZ2	1.77	0.49
1:B:29:ILE:CD1	1:B:62:MET:HG2	2.42	0.49
1:D:229:GLY:O	1:D:248:VAL:HG23	2.13	0.49
1:B:125:LEU:HB3	1:B:327:ILE:HD11	1.95	0.49
1:D:228:ILE:HG23	1:D:258:ILE:HD11	1.93	0.49
1:A:75:ILE:HA	1:A:187:TYR:O	2.13	0.49
1:B:179:LEU:HD23	1:B:190:MET:HE3	1.93	0.49
1:C:263:VAL:HG12	1:C:272:LYS:HG3	1.94	0.49
1:C:87:THR:HG21	1:C:224:GLU:OE2	2.13	0.49
1:C:191:GLY:HA3	1:C:223:ASP:O	2.13	0.49
1:C:170:ARG:HA	1:C:174:ASN:ND2	2.28	0.49
1:D:231:THR:N	1:D:246:LEU:O	2.45	0.49
1:A:3:ILE:CD1	1:A:37:LEU:HD13	2.41	0.48
1:D:41:ILE:O	1:D:45:LEU:HB2	2.13	0.48
1:C:204:SER:O	1:C:208:LEU:HD23	2.12	0.48
1:C:299:LEU:O	1:C:300:ASP:HB2	2.12	0.48
1:A:114:GLY:N	3:A:401:HOH:O	2.46	0.48
1:A:191:GLY:HA3	1:A:223:ASP:O	2.13	0.48
1:A:256:ILE:HD12	1:A:256:ILE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ASP:HA	1:B:48:LYS:HZ2	1.77	0.48
1:A:113:SER:HB2	3:A:401:HOH:O	2.13	0.48
1:A:171:THR:N	1:A:174:ASN:ND2	2.51	0.48
1:C:2:ASN:CG	1:C:5:GLU:HB2	2.34	0.48
1:C:88:VAL:HG13	1:C:90:VAL:HG13	1.94	0.48
1:D:191:GLY:HA3	1:D:223:ASP:O	2.13	0.48
1:D:216:VAL:HG12	1:D:233:MET:HG3	1.94	0.48
1:D:265:SER:HG	1:D:268:ASP:CG	2.17	0.48
1:C:213:ILE:HG23	1:C:236:VAL:HB	1.96	0.48
1:D:318:LYS:HD2	1:D:318:LYS:N	2.28	0.48
1:B:323:LEU:HB3	1:B:335:LYS:NZ	2.29	0.48
1:A:40:ALA:HB1	1:D:43:VAL:HG21	1.94	0.48
1:A:195:LYS:O	1:A:198:LEU:HB2	2.14	0.48
1:B:15:ASP:HA	1:B:48:LYS:NZ	2.29	0.47
1:B:29:ILE:CG2	1:B:156:ALA:HB1	2.39	0.47
1:B:1:MET:O	1:B:1:MET:HG3	2.14	0.47
1:B:177:GLY:N	1:B:178:PRO:HD2	2.30	0.47
1:B:213:ILE:CG2	1:B:236:VAL:HB	2.44	0.47
1:C:13:LYS:CA	1:C:48:LYS:HG3	2.42	0.47
1:C:192:VAL:HG22	1:C:201:LEU:HD12	1.95	0.47
1:D:208:LEU:O	1:D:209:ASP:CB	2.62	0.47
1:D:311:TYR:O	1:D:315:LEU:HG	2.14	0.47
1:A:50:GLU:CD	1:A:50:GLU:H	2.16	0.47
1:A:280:LYS:O	1:A:281:ASP:HB2	2.14	0.47
1:B:40:ALA:CB	1:C:43:VAL:HG21	2.42	0.47
1:B:62:MET:HE1	1:B:176:LEU:HD13	1.96	0.47
1:B:216:VAL:HG12	1:B:233:MET:CB	2.35	0.47
1:D:220:PRO:HD3	1:D:226:SER:HG	1.78	0.47
1:D:253:ILE:HG22	1:D:254:SER:H	1.78	0.47
1:B:1:MET:O	1:B:1:MET:CG	2.63	0.47
1:B:76:ASP:OD1	1:B:106:LYS:HA	2.14	0.47
1:D:247:ASN:N	1:D:250:ASP:OD2	2.46	0.47
1:D:328:SER:HA	1:D:333:VAL:HG13	1.96	0.47
1:A:342:LYS:HE2	1:A:342:LYS:CA	2.39	0.47
1:B:223:ASP:C	1:B:224:GLU:HG3	2.35	0.47
1:C:50:GLU:CD	1:C:50:GLU:H	2.18	0.47
1:C:115:LYS:HE2	1:C:115:LYS:H	1.80	0.47
1:C:148:LEU:HD13	1:C:182:PRO:HB2	1.97	0.47
1:D:278:LEU:HD13	1:D:345:GLY:HA2	1.97	0.47
1:A:276:ALA:HA	3:A:386:HOH:O	2.14	0.46
1:B:102:ASN:CG	1:B:103:PRO:HD2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LYS:HD2	1:B:115:LYS:H	1.80	0.46
1:B:164:ARG:NH1	1:B:173:PHE:HB3	2.29	0.46
1:D:214:ILE:HD12	1:D:298:ALA:HB2	1.97	0.46
1:B:55:ILE:HD11	1:B:200:LEU:HD21	1.96	0.46
1:B:59:ALA:O	1:B:63:ARG:HG3	2.15	0.46
1:B:271:ILE:HG12	1:B:342:LYS:HE3	1.96	0.46
1:D:115:LYS:HD2	1:D:115:LYS:N	2.30	0.46
1:D:219:GLU:H	1:D:226:SER:HB2	1.79	0.46
1:A:170:ARG:HA	1:A:174:ASN:ND2	2.30	0.46
1:C:91:SER:OG	1:C:106:LYS:NZ	2.48	0.46
1:C:258:ILE:O	1:C:258:ILE:HD13	2.15	0.46
1:B:135:ARG:HG3	1:B:135:ARG:NH1	2.30	0.46
1:B:247:ASN:ND2	1:B:249:THR:HB	2.28	0.46
1:A:134:GLU:OE1	1:A:134:GLU:N	2.33	0.46
1:A:160:VAL:O	1:A:160:VAL:CG1	2.61	0.46
1:A:209:ASP:OD1	1:A:238:LYS:NZ	2.48	0.46
1:A:223:ASP:C	1:A:224:GLU:HG3	2.36	0.46
1:A:43:VAL:HG21	1:D:40:ALA:HB1	1.98	0.46
1:C:344:SER:O	1:C:345:GLY:C	2.54	0.46
1:B:44:ALA:HA	1:C:47:MET:SD	2.56	0.46
1:D:304:ASP:OD1	1:D:306:ARG:N	2.46	0.46
1:D:173:PHE:HA	1:D:176:LEU:HD12	1.98	0.46
1:D:226:SER:HA	1:D:227:PRO:HD3	1.67	0.46
1:D:1:MET:CE	1:D:3:ILE:HD13	2.45	0.46
1:D:230:ASN:HA	1:D:246:LEU:O	2.15	0.46
1:D:263:VAL:HG12	1:D:264:ASN:N	2.31	0.46
1:A:135:ARG:HG3	1:A:135:ARG:NH1	2.30	0.45
1:C:282:GLU:O	1:C:286:GLU:HG3	2.15	0.45
1:D:181:ASN:HD21	1:D:183:ALA:HB3	1.81	0.45
1:D:111:ALA:HB2	1:D:117:GLY:N	2.30	0.45
1:D:306:ARG:HG3	1:D:306:ARG:NH1	2.31	0.45
1:A:342:LYS:HA	1:A:342:LYS:CE	2.41	0.45
1:D:113:SER:O	1:D:115:LYS:HD2	2.16	0.45
1:A:62:MET:HE1	1:A:176:LEU:HD13	1.98	0.45
1:C:71:VAL:HG12	1:C:74:ALA:HB2	1.98	0.45
1:C:75:ILE:HA	1:C:187:TYR:O	2.16	0.45
1:B:271:ILE:HG22	1:B:275:ARG:HD2	1.98	0.45
1:D:234:LYS:NZ	1:D:243:GLU:HG3	2.31	0.45
1:D:278:LEU:CD1	1:D:345:GLY:HA2	2.47	0.45
1:D:50:GLU:H	1:D:50:GLU:CD	2.20	0.45
1:D:302:VAL:HG11	1:D:308:GLY:CA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASN:OD1	1:C:103:PRO:HD2	2.16	0.45
1:C:292:THR:HG22	1:C:296:LEU:HD22	1.98	0.45
1:B:171:THR:N	1:B:174:ASN:ND2	2.50	0.45
1:D:9:LYS:HG3	1:D:14:SER:OG	2.17	0.45
1:B:74:ALA:HA	1:B:103:PRO:HG2	1.99	0.45
1:D:134:GLU:H	1:D:134:GLU:CD	2.15	0.45
1:B:6:ILE:HG21	1:B:24:LEU:HD22	1.98	0.45
1:B:227:PRO:HG2	1:B:228:ILE:HG23	1.99	0.44
1:B:313:ASP:O	1:B:316:ILE:HG22	2.17	0.44
1:C:38:VAL:O	1:C:42:LEU:HG	2.17	0.44
1:D:208:LEU:HD13	1:D:208:LEU:HA	1.77	0.44
1:B:342:LYS:HD2	1:B:342:LYS:H	1.81	0.44
1:D:181:ASN:ND2	1:D:183:ALA:H	2.15	0.44
1:B:140:VAL:O	1:B:144:ASN:HA	2.16	0.44
1:C:225:VAL:HG21	1:C:294:VAL:HG21	1.98	0.44
1:C:181:ASN:HD22	1:C:185:ALA:H	1.65	0.44
1:D:285:ALA:O	1:D:289:LYS:HG3	2.16	0.44
1:A:256:ILE:HG23	1:A:257:PRO:HD2	1.99	0.44
1:C:45:LEU:HD12	1:C:45:LEU:HA	1.88	0.44
1:C:302:VAL:CG1	1:C:307:GLU:HB3	2.48	0.44
1:A:133:PRO:HG2	1:A:134:GLU:OE1	2.17	0.44
1:B:253:ILE:CG2	1:B:254:SER:N	2.73	0.44
1:D:316:ILE:O	1:D:319:SER:HB2	2.18	0.44
1:C:280:LYS:HE3	1:C:345:GLY:HA3	1.99	0.44
1:D:228:ILE:CG1	1:D:229:GLY:N	2.81	0.43
1:D:268:ASP:O	1:D:272:LYS:HG3	2.18	0.43
1:A:329:MET:HA	1:A:329:MET:CE	2.48	0.43
1:B:102:ASN:OD1	1:B:103:PRO:HD2	2.18	0.43
1:B:247:ASN:ND2	1:B:249:THR:H	2.16	0.43
1:D:289:LYS:HE2	1:D:313:ASP:OD1	2.18	0.43
1:A:40:ALA:HB2	1:D:167:LEU:HD21	2.00	0.43
1:C:135:ARG:HG3	1:C:135:ARG:HH11	1.83	0.43
1:A:75:ILE:HG12	1:A:76:ASP:N	2.34	0.43
1:B:3:ILE:CD1	1:B:41:ILE:HD11	2.46	0.43
1:C:48:LYS:NZ	1:C:54:GLU:CD	2.71	0.43
1:C:192:VAL:CG1	1:C:197:HIS:HB2	2.49	0.43
1:A:134:GLU:H	1:A:134:GLU:CD	2.12	0.43
1:B:155:PRO:O	1:B:158:LYS:HG2	2.18	0.43
1:C:62:MET:CE	1:C:180:THR:HG21	2.49	0.43
1:D:263:VAL:HG12	1:D:265:SER:H	1.83	0.43
1:A:88:VAL:HG23	1:A:269:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ARG:NH1	1:B:174:ASN:CB	2.82	0.43
1:C:115:LYS:H	1:C:115:LYS:CE	2.32	0.43
1:D:222:ILE:HG22	1:D:224:GLU:H	1.84	0.43
1:A:64:GLU:HG3	3:A:371:HOH:O	2.18	0.43
1:A:188:GLN:HG3	1:A:189:LEU:N	2.34	0.43
1:A:340:VAL:O	1:A:341:VAL:C	2.58	0.42
1:C:301:ARG:HG3	1:C:301:ARG:HH21	1.84	0.42
1:B:9:LYS:HG2	1:B:14:SER:OG	2.19	0.42
1:C:3:ILE:CG2	1:C:41:ILE:HD11	2.49	0.42
1:C:230:ASN:HA	1:C:246:LEU:O	2.19	0.42
1:C:172:ILE:O	1:C:176:LEU:HG	2.20	0.42
1:D:230:ASN:HA	1:D:247:ASN:HA	2.01	0.42
1:A:71:VAL:HG12	1:A:74:ALA:HB2	2.00	0.42
1:B:215:LEU:O	1:B:233:MET:HA	2.20	0.42
1:D:310:GLU:O	1:D:313:ASP:HB2	2.19	0.42
1:B:101:VAL:O	1:B:102:ASN:HB2	2.20	0.42
1:C:181:ASN:HA	1:C:182:PRO:HD3	1.87	0.42
1:C:187:TYR:HA	1:C:212:LYS:O	2.19	0.42
1:B:62:MET:HE1	1:B:176:LEU:CD1	2.50	0.42
1:D:114:GLY:O	1:D:265:SER:HA	2.20	0.42
1:B:90:VAL:HG11	1:B:287:PHE:CD2	2.55	0.42
1:B:137:LYS:O	1:B:141:ASN:ND2	2.53	0.42
1:B:154:HIS:HB3	1:B:157:MET:HG2	2.02	0.42
1:B:234:LYS:NZ	1:B:243:GLU:HG2	2.34	0.42
1:B:239:ARG:NH1	1:B:240:GLY:C	2.73	0.42
1:C:111:ALA:CB	1:C:117:GLY:H	2.32	0.42
1:D:246:LEU:HD21	1:D:251:PHE:CZ	2.54	0.42
1:A:43:VAL:HG21	1:D:40:ALA:CB	2.50	0.42
1:A:213:ILE:CG2	1:A:236:VAL:HB	2.48	0.42
1:B:135:ARG:O	1:B:139:LEU:HG	2.20	0.42
1:A:230:ASN:HA	1:A:246:LEU:O	2.20	0.41
1:A:259:GLU:CD	1:A:259:GLU:H	2.23	0.41
1:B:336:LEU:HD22	3:B:433:HOH:O	2.18	0.41
1:B:336:LEU:C	1:B:339:ILE:HG22	2.41	0.41
1:D:322:LYS:HD2	1:D:325:GLU:OE2	2.20	0.41
1:A:107:HIS:NE2	1:A:150:ALA:HB2	2.35	0.41
1:A:163:VAL:HG23	3:A:358:HOH:O	2.20	0.41
1:D:1:MET:HE1	1:D:3:ILE:HD13	2.02	0.41
1:D:77:THR:HG22	1:D:189:LEU:HB3	2.02	0.41
1:D:144:ASN:HD22	1:D:144:ASN:HA	1.62	0.41
1:B:3:ILE:CD1	1:B:33:VAL:HG13	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:ILE:HG23	1:D:41:ILE:HD11	2.01	0.41
1:D:113:SER:O	1:D:115:LYS:N	2.50	0.41
1:B:233:MET:CG	1:B:244:VAL:HB	2.47	0.41
1:C:3:ILE:HG23	1:C:41:ILE:HD11	2.02	0.41
1:C:74:ALA:HA	1:C:103:PRO:HG2	2.02	0.41
1:B:111:ALA:HB2	1:B:117:GLY:N	2.36	0.41
1:B:214:ILE:HD12	1:B:298:ALA:HB2	2.03	0.41
1:D:253:ILE:CG2	1:D:254:SER:N	2.79	0.41
1:A:36:ILE:HD13	1:D:163:VAL:HA	2.02	0.41
1:C:144:ASN:HD22	1:C:144:ASN:HA	1.62	0.41
1:C:177:GLY:N	1:C:178:PRO:HD2	2.36	0.41
1:C:190:MET:CE	1:C:201:LEU:HD13	2.50	0.41
1:D:242:GLU:HG2	1:D:244:VAL:HG23	2.02	0.41
1:B:29:ILE:HD13	1:B:62:MET:HG2	2.00	0.41
1:B:66:ALA:HB2	1:B:154:HIS:CE1	2.55	0.41
1:B:181:ASN:HD22	1:B:184:ASN:N	2.19	0.41
1:C:160:VAL:HG12	1:C:164:ARG:HG3	2.03	0.41
1:C:181:ASN:ND2	1:C:183:ALA:H	2.19	0.41
1:C:209:ASP:HA	3:C:529:HOH:O	2.20	0.41
1:A:246:LEU:HD12	1:A:250:ASP:OD2	2.20	0.41
1:B:52:LYS:O	1:B:56:VAL:HG23	2.21	0.41
1:C:125:LEU:HB3	1:C:327:ILE:HD11	2.03	0.41
1:C:286:GLU:HA	1:C:289:LYS:HE3	2.03	0.41
1:C:337:LYS:O	1:C:341:VAL:HG23	2.21	0.41
1:D:24:LEU:HD11	1:D:41:ILE:HD13	2.03	0.41
1:D:275:ARG:HB2	1:D:343:SER:OG	2.21	0.41
1:A:332:ASP:OD1	1:A:334:THR:OG1	2.39	0.41
1:B:2:ASN:HB3	1:B:5:GLU:OE2	2.21	0.41
1:B:181:ASN:ND2	1:B:185:ALA:H	2.19	0.41
1:B:323:LEU:HD23	1:B:335:LYS:CE	2.48	0.41
1:C:280:LYS:HE3	1:C:345:GLY:CA	2.50	0.41
1:D:181:ASN:HA	1:D:182:PRO:HD3	1.91	0.41
1:C:140:VAL:O	1:C:144:ASN:HA	2.21	0.40
1:A:47:MET:HE3	1:D:13:LYS:HE3	2.03	0.40
1:A:62:MET:HE1	1:A:176:LEU:CD1	2.51	0.40
1:A:70:ASP:OD1	1:A:72:PRO:HD3	2.20	0.40
1:A:302:VAL:HG11	1:A:308:GLY:HA2	2.03	0.40
1:B:338:THR:HG22	1:B:342:LYS:CE	2.51	0.40
1:D:140:VAL:O	1:D:144:ASN:HA	2.22	0.40
1:A:286:GLU:OE1	1:A:309:TYR:OH	2.38	0.40
1:C:34:PRO:HD2	1:C:37:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:PHE:CE1	1:C:305:PHE:HB3	2.57	0.40
1:D:282:GLU:HG3	1:D:283:HIS:N	2.36	0.40
1:B:47:MET:SD	1:C:44:ALA:HA	2.62	0.40
1:C:48:LYS:HE2	1:C:48:LYS:HB3	1.92	0.40
1:D:236:VAL:HB	1:D:241:ILE:HG12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ILE:CD1	1:C:67:ILE:CD1[2_657]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	336/345 (97%)	317 (94%)	15 (4%)	4 (1%)	13	13
1	B	336/345 (97%)	314 (94%)	19 (6%)	3 (1%)	17	20
1	C	337/345 (98%)	315 (94%)	19 (6%)	3 (1%)	17	20
1	D	343/345 (99%)	324 (94%)	16 (5%)	3 (1%)	17	20
All	All	1352/1380 (98%)	1270 (94%)	69 (5%)	13 (1%)	15	16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ASP
1	A	113	SER
1	A	115	LYS
1	B	330	ASN
1	C	114	GLY

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Mol	Chain	Res	Type
1	C	115	LYS
1	D	114	GLY
1	D	209	ASP
1	D	344	SER
1	A	221	GLY
1	B	221	GLY
1	C	221	GLY
1	B	333	VAL

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	287/289 (99%)	270 (94%)	17 (6%)	19	25
1	B	287/289 (99%)	274 (96%)	13 (4%)	27	36
1	C	287/289 (99%)	277 (96%)	10 (4%)	36	47
1	D	289/289 (100%)	275 (95%)	14 (5%)	25	34
All	All	1150/1156 (100%)	1096 (95%)	54 (5%)	26	35

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

Mol	Chain	Res	Type
1	A	45	LEU
1	A	100	LEU
1	A	115	LYS
1	A	134	GLU
1	A	144	ASN
1	A	149	PHE
1	A	158	LYS
1	A	162	ASN
1	A	208	LEU
1	A	220	PRO
1	A	282	GLU
1	A	296	LEU
1	A	306	ARG

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Mol	Chain	Res	Type
1	A	311	TYR
1	A	325	GLU
1	A	329	MET
1	A	342	LYS
1	B	100	LEU
1	B	115	LYS
1	B	125	LEU
1	B	134	GLU
1	B	144	ASN
1	B	184	ASN
1	B	198	LEU
1	B	199	ASP
1	B	239	ARG
1	B	258	ILE
1	B	296	LEU
1	B	313	ASP
1	B	338	THR
1	C	97	LEU
1	C	100	LEU
1	C	115	LYS
1	C	144	ASN
1	C	212	LYS
1	C	224	GLU
1	C	243	GLU
1	C	258	ILE
1	C	296	LEU
1	C	334	THR
1	D	90	VAL
1	D	97	LEU
1	D	100	LEU
1	D	115	LYS
1	D	125	LEU
1	D	144	ASN
1	D	193	PHE
1	D	198	LEU
1	D	208	LEU
1	D	236	VAL
1	D	255	PRO
1	D	269	SER
1	D	306	ARG
1	D	313	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	144	ASN
1	A	162	ASN
1	A	174	ASN
1	A	247	ASN
1	B	4	ASN
1	B	102	ASN
1	B	141	ASN
1	B	151	GLN
1	B	162	ASN
1	B	174	ASN
1	B	181	ASN
1	B	188	GLN
1	B	211	ASN
1	B	247	ASN
1	B	283	HIS
1	C	144	ASN
1	C	151	GLN
1	C	162	ASN
1	C	174	ASN
1	C	181	ASN
1	C	197	HIS
1	D	144	ASN
1	D	151	GLN
1	D	162	ASN
1	D	174	ASN
1	D	181	ASN
1	D	283	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	BE2	D	602	-	10,10,10	1.34	1 (10%)	13,13,13	1.01	1 (7%)
2	BE2	C	502	-	10,10,10	1.34	2 (20%)	13,13,13	1.06	2 (15%)
2	BE2	D	601	-	10,10,10	1.30	1 (10%)	13,13,13	0.91	0
2	BE2	B	402	-	10,10,10	1.37	2 (20%)	13,13,13	0.97	0
2	BE2	A	346	-	10,10,10	1.32	2 (20%)	13,13,13	0.97	0
2	BE2	B	401	-	10,10,10	1.46	2 (20%)	13,13,13	1.06	2 (15%)
2	BE2	C	501	-	10,10,10	1.35	1 (10%)	13,13,13	0.91	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	BE2	D	602	-	-	0/4/4/4	0/1/1/1
2	BE2	C	502	-	-	0/4/4/4	0/1/1/1
2	BE2	D	601	-	-	0/4/4/4	0/1/1/1
2	BE2	B	402	-	-	0/4/4/4	0/1/1/1
2	BE2	A	346	-	-	0/4/4/4	0/1/1/1
2	BE2	B	401	-	-	0/4/4/4	0/1/1/1
2	BE2	C	501	-	-	0/4/4/4	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	BE2	C6-C1	2.94	1.44	1.39
2	B	402	BE2	C6-C1	2.80	1.44	1.39
2	C	501	BE2	C6-C1	2.76	1.44	1.39
2	D	602	BE2	C6-C1	2.70	1.44	1.39
2	A	346	BE2	C6-C1	2.60	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	BE2	C6-C1	2.58	1.44	1.39
2	D	601	BE2	C6-C1	2.37	1.43	1.39
2	C	502	BE2	C1-CA	2.33	1.45	1.41
2	B	401	BE2	C1-CA	2.24	1.45	1.41
2	B	402	BE2	C1-CA	2.05	1.44	1.41
2	A	346	BE2	C1-CA	2.01	1.44	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	602	BE2	C3-CA-C1	2.23	120.25	118.10
2	C	502	BE2	C3-CA-N	-2.13	116.00	120.13
2	C	502	BE2	C3-CA-C1	2.11	120.14	118.10
2	B	401	BE2	C3-CA-C1	2.04	120.08	118.10
2	B	401	BE2	C3-CA-N	-2.01	116.23	120.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	602	BE2	1	0
2	C	502	BE2	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(Å²)	Q<0.9
1	A	340/345 (98%)	-0.01	7 (2%)	63	60	36, 53, 70, 84	0
1	B	340/345 (98%)	0.20	11 (3%)	47	44	37, 59, 89, 109	0
1	C	341/345 (98%)	0.10	14 (4%)	37	34	37, 56, 78, 95	0
1	D	345/345 (100%)	0.22	12 (3%)	44	40	35, 59, 89, 97	0
All	All	1366/1380 (98%)	0.13	44 (3%)	47	44	35, 56, 83, 109	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	345	GLY	10.3
1	D	114	GLY	8.7
1	D	345	GLY	6.6
1	B	114	GLY	6.2
1	B	112	VAL	5.8
1	D	85	LEU	5.4
1	B	111	ALA	4.8
1	D	115	LYS	4.5
1	B	343	SER	4.4
1	A	113	SER	4.4
1	C	85	LEU	4.3
1	D	112	VAL	4.2
1	C	115	LYS	4.2
1	B	115	LYS	4.0
1	B	113	SER	4.0
1	C	344	SER	3.8
1	C	112	VAL	3.6
1	C	114	GLY	3.3
1	D	225	VAL	3.2
1	A	114	GLY	3.1
1	D	239	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	83	ASP	2.9
1	D	113	SER	2.9
1	B	337	LYS	2.8
1	C	303	GLY	2.8
1	A	116	SER	2.8
1	D	42	LEU	2.7
1	C	86	GLY	2.7
1	B	1	MET	2.7
1	A	280	LYS	2.6
1	D	306	ARG	2.6
1	A	1	MET	2.5
1	B	55	ILE	2.5
1	B	332	ASP	2.4
1	D	215	LEU	2.3
1	A	193	PHE	2.3
1	C	84	GLY	2.3
1	B	41	ILE	2.2
1	C	41	ILE	2.2
1	C	239	ARG	2.2
1	A	112	VAL	2.2
1	C	290	ILE	2.1
1	C	42	LEU	2.1
1	C	213	ILE	2.0

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 monosaccharides 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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BE2	C	502	10/10	0.87	0.19	88,88,90,91	0
2	BE2	A	346	10/10	0.88	0.19	57,59,63,65	0
2	BE2	D	602	10/10	0.90	0.17	60,61,63,65	0
2	BE2	B	401	10/10	0.92	0.14	65,66,69,72	0
2	BE2	B	402	10/10	0.93	0.18	60,63,65,67	0
2	BE2	C	501	10/10	0.94	0.28	57,59,62,65	0
2	BE2	D	601	10/10	0.96	0.16	35,38,47,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.