



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:13 PM GMT

PDB ID : 1PMO
Title : Crystal structure of Escherichia coli GadB (neutral pH)
Authors : Capitani, G.; De Biase, D.; Aurizi, C.; Gut, H.; Bossa, F.; Grutter, M.G.
Deposited on : 2003-06-11
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

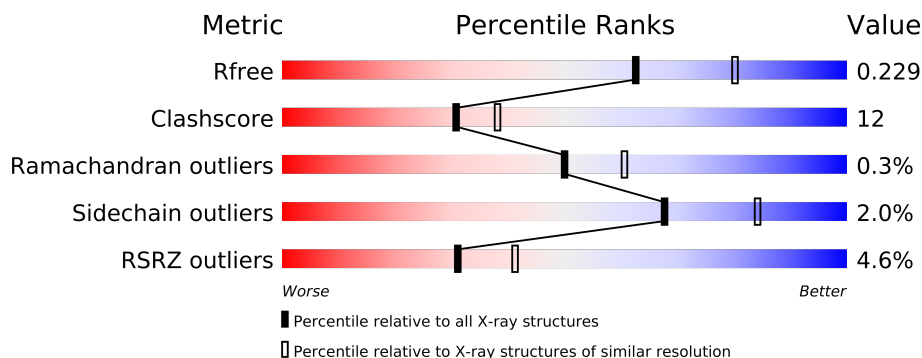
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	466	
1	B	466	
1	C	466	
1	D	466	
1	E	466	
1	F	466	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	TRS	A	3236	-	X
3	TRS	A	3241	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
3	TRS	A	3251	-	X
3	TRS	B	3237	-	X
3	TRS	B	3242	-	X
3	TRS	C	3243	-	X
3	TRS	C	3250	-	X
3	TRS	C	3252	-	X
3	TRS	D	3238	-	X
3	TRS	D	3244	-	X
3	TRS	D	3245	-	X
3	TRS	E	3239	-	X
3	TRS	E	3246	-	X
3	TRS	E	3247	-	X
3	TRS	E	3253	-	X
3	TRS	F	3240	-	X
3	TRS	F	3248	-	X
3	TRS	F	3249	-	X

2 Entry composition i

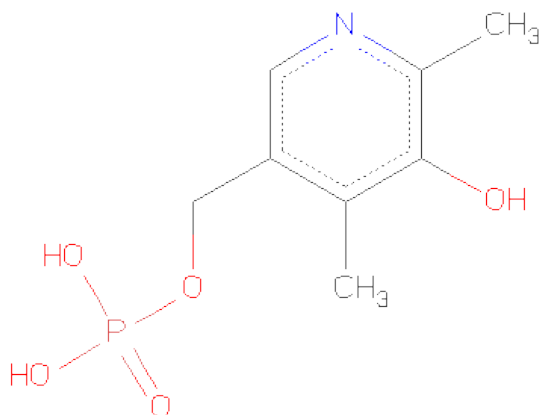
There are 4 unique types of molecules in this entry. The entry contains 23202 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glutamate decarboxylase beta.

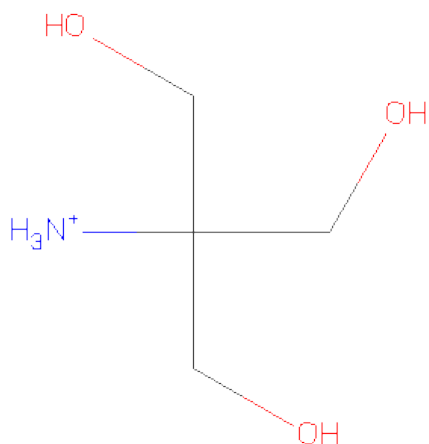
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3616	2308	617	667	24			
1	B	463	Total	C	N	O	S	0	0	0
			3681	2347	630	680	24			
1	C	454	Total	C	N	O	S	0	0	0
			3607	2303	616	664	24			
1	D	454	Total	C	N	O	S	0	0	0
			3607	2303	616	664	24			
1	E	463	Total	C	N	O	S	0	0	0
			3681	2347	630	680	24			
1	F	454	Total	C	N	O	S	0	0	0
			3607	2303	616	664	24			

- Molecule 2 is (5-HYDROXY-4,6-DIMETHYLPYRIDIN-3-YL)METHYLDIHYDROGEN PHOSPHATE (three-letter code: PLR) (formula: C₈H₁₂NO₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

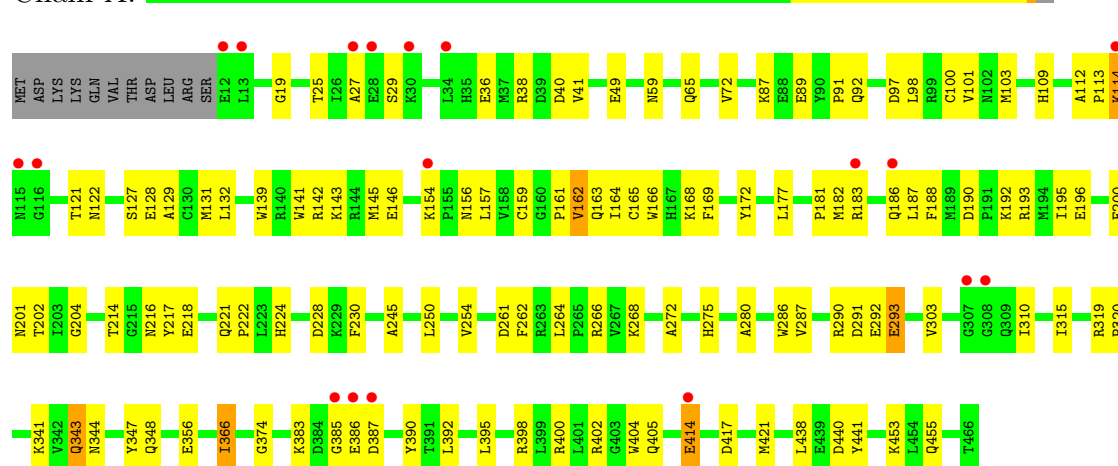
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	188	Total	O	0	0
			188	188		
4	B	190	Total	O	0	0
			190	190		
4	C	207	Total	O	0	0
			207	207		
4	D	187	Total	O	0	0
			187	187		
4	E	208	Total	O	0	0
			208	208		
4	F	189	Total	O	0	0
			189	189		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

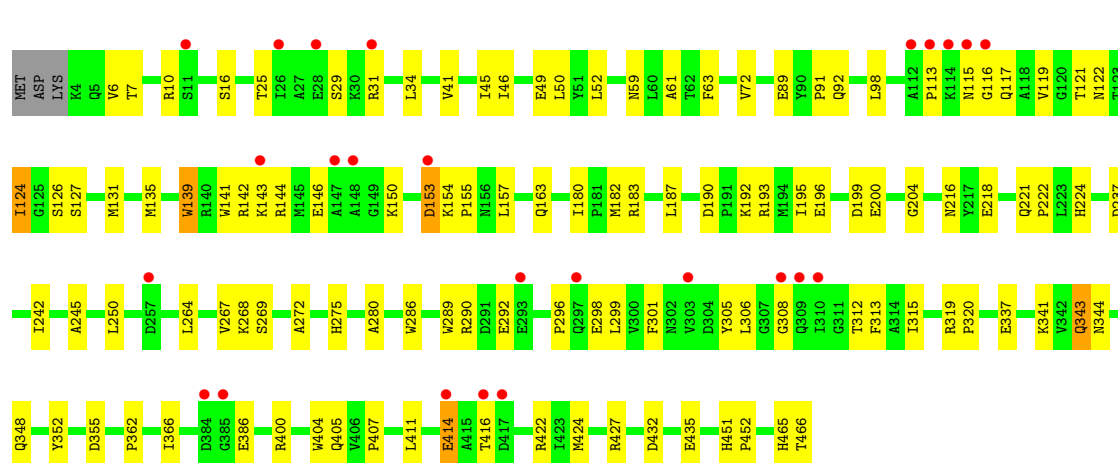
• Molecule 1: Glutamate decarboxylase beta

Chain A:



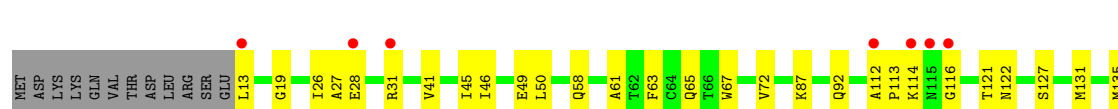
• Molecule 1: Glutamate decarboxylase beta

Chain B:

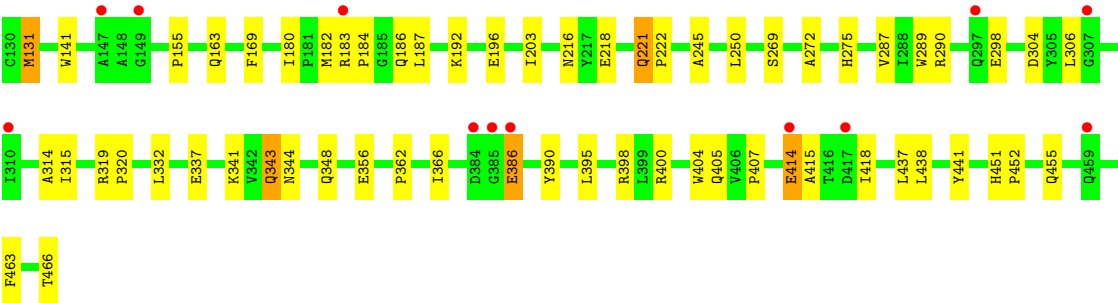


• Molecule 1: Glutamate decarboxylase beta

Chain C:







4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	116.00Å 116.00Å 207.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.30) 98.8 (20.00-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.233 0.196 , 0.229	Depositor DCC
R_{free} test set	2749 reflections (2.02%)	DCC
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 36.3	EDS
Estimated twinning fraction	0.003 for -h,-k,l 0.025 for h,-h-k,-l 0.016 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 136306 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23202	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 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.37	0/3710	0.61	1/5028 (0.0%)
1	B	0.36	0/3775	0.60	1/5115 (0.0%)
1	C	0.38	0/3701	0.60	1/5016 (0.0%)
1	D	0.36	0/3701	0.60	1/5016 (0.0%)
1	E	0.36	0/3775	0.61	1/5115 (0.0%)
1	F	0.38	0/3701	0.60	1/5016 (0.0%)
All	All	0.37	0/22363	0.60	6/30306 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	GLU	N-CA-C	-5.37	96.49	111.00
1	F	218	GLU	N-CA-C	-5.36	96.53	111.00
1	C	218	GLU	N-CA-C	-5.29	96.70	111.00
1	B	218	GLU	N-CA-C	-5.26	96.78	111.00
1	E	218	GLU	N-CA-C	-5.24	96.86	111.00
1	A	218	GLU	N-CA-C	-5.14	97.12	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3616	0	3516	114	0
1	B	3681	0	3586	84	0
1	C	3607	0	3510	87	0
1	D	3607	0	3510	83	0
1	E	3681	0	3586	97	0
1	F	3607	0	3510	76	0
2	A	15	0	9	0	0
2	B	15	0	9	1	0
2	C	15	0	9	1	0
2	D	15	0	9	0	0
2	E	15	0	9	0	0
2	F	15	0	9	1	0
3	A	24	0	36	12	0
3	B	16	0	24	7	0
3	C	24	0	36	18	0
3	D	24	0	36	9	0
3	E	32	0	48	14	0
3	F	24	0	36	17	0
4	A	188	0	0	7	0
4	B	190	0	0	2	0
4	C	207	0	0	5	0
4	D	187	0	0	6	0
4	E	208	0	0	5	0
4	F	189	0	0	5	0
All	All	23202	0	21488	512	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (512) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:65:GLN:HB3	3:A:3236:TRS:H31	1.20	1.11
1:F:250:LEU:HD23	1:F:343:GLN:HG3	1.42	1.01
1:A:250:LEU:HD23	1:A:343:GLN:HG3	1.44	0.98
1:B:250:LEU:HD23	1:B:343:GLN:HG3	1.46	0.97
1:C:436:LEU:HD11	3:C:3252:TRS:H21	1.47	0.96
1:A:183:ARG:HG2	1:A:414:GLU:HB2	1.47	0.94
1:F:72:VAL:HG21	3:F:3240:TRS:H12	1.54	0.88
1:B:190:ASP:OD1	1:B:193:ARG:HD3	1.76	0.85
1:D:121:THR:OG1	3:D:3244:TRS:H11	1.76	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:250:LEU:HD23	1:C:343:GLN:HG3	1.57	0.84
1:C:183:ARG:HD2	1:C:186:GLN:HE21	1.40	0.84
1:B:183:ARG:HG2	1:B:414:GLU:HB2	1.59	0.84
1:A:91:PRO:HB2	3:C:3252:TRS:H12	1.60	0.82
1:C:281:PRO:HB3	3:C:3250:TRS:H22	1.62	0.82
1:C:362:PRO:HB2	1:C:386:GLU:HG2	1.64	0.81
1:E:49:GLU:O	1:F:92:GLN:HG2	1.83	0.79
1:E:427:ARG:HH21	3:E:3239:TRS:H12	1.47	0.78
1:A:114:LYS:HD2	1:A:114:LYS:H	1.49	0.78
1:D:190:ASP:OD1	1:D:193:ARG:HD3	1.82	0.78
1:A:190:ASP:OD1	1:A:193:ARG:HD3	1.84	0.77
1:D:114:LYS:HD2	1:D:114:LYS:H	1.48	0.77
1:A:65:GLN:HB3	3:A:3236:TRS:C3	2.09	0.77
1:C:72:VAL:HG11	3:C:3250:TRS:H12	1.66	0.77
1:D:362:PRO:HB2	1:D:386:GLU:HG2	1.67	0.77
1:D:65:GLN:HB3	3:D:3238:TRS:N	2.00	0.76
1:E:92:GLN:HG2	1:F:49:GLU:O	1.87	0.74
1:D:221:GLN:HB3	1:D:222:PRO:HD3	1.69	0.74
1:E:362:PRO:HB2	1:E:386:GLU:HG2	1.70	0.73
1:E:411:LEU:O	1:E:416:THR:HA	1.89	0.73
1:C:183:ARG:HB2	1:C:186:GLN:HG3	1.69	0.73
1:E:127:SER:O	1:E:131:MET:HG2	1.88	0.73
1:E:5:GLN:HG3	1:E:10:ARG:HD2	1.70	0.73
1:A:214:THR:CG2	1:A:366:ILE:HD11	2.18	0.73
1:F:183:ARG:HE	1:F:414:GLU:HG2	1.54	0.73
1:E:427:ARG:NH2	3:E:3239:TRS:H12	2.04	0.72
1:A:221:GLN:HB3	1:A:222:PRO:HD3	1.70	0.72
1:C:183:ARG:HD2	1:C:186:GLN:NE2	2.02	0.72
1:B:341:LYS:HE2	1:C:19:GLY:O	1.88	0.72
1:B:124:ILE:CD1	1:B:319:ARG:HD2	2.19	0.72
1:D:390:TYR:HA	1:D:455:GLN:HG3	1.72	0.72
1:C:114:LYS:HZ2	1:C:292:GLU:HG2	1.55	0.71
1:F:356:GLU:HG2	1:F:438:LEU:HD13	1.71	0.71
1:A:65:GLN:CB	3:A:3236:TRS:H31	2.11	0.71
1:C:121:THR:HA	3:C:3243:TRS:H12	1.72	0.71
1:E:190:ASP:OD1	1:E:193:ARG:HD3	1.91	0.71
1:A:91:PRO:CB	3:C:3252:TRS:H12	2.20	0.71
1:E:7:THR:HA	1:E:10:ARG:HD3	1.71	0.71
1:D:242:ILE:HD11	1:D:267:VAL:HG22	1.73	0.71
1:E:315:ILE:HG21	1:F:315:ILE:HD13	1.73	0.70
1:D:65:GLN:HB3	3:D:3238:TRS:HN2	1.56	0.70
1:E:183:ARG:HH21	1:E:414:GLU:HG2	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:84:TRP:HZ2	3:D:3244:TRS:H12	1.57	0.69
1:A:341:LYS:HE2	1:F:19:GLY:O	1.91	0.69
1:F:121:THR:OG1	3:F:3248:TRS:H31	1.92	0.69
1:E:364:GLU:OE1	1:E:381:LYS:HE3	1.93	0.68
1:B:362:PRO:HB2	1:B:386:GLU:HG2	1.75	0.68
1:F:127:SER:O	1:F:131:MET:HG2	1.94	0.68
1:F:72:VAL:HG21	3:F:3240:TRS:C1	2.24	0.68
1:F:250:LEU:CD2	1:F:343:GLN:HG3	2.22	0.68
1:C:92:GLN:HG2	1:D:49:GLU:O	1.93	0.68
1:A:164:ILE:HD12	1:A:165:CYS:N	2.07	0.67
1:C:49:GLU:O	1:D:92:GLN:HG2	1.94	0.67
1:D:422:ARG:HD2	4:D:3284:HOH:O	1.95	0.67
1:A:291:ASP:OD1	1:A:293:GLU:HG2	1.95	0.67
1:D:19:GLY:O	1:E:341:LYS:HE2	1.95	0.66
1:F:183:ARG:HG3	1:F:184:PRO:HD2	1.78	0.66
1:C:242:ILE:HD13	1:C:267:VAL:HG13	1.77	0.66
1:D:84:TRP:CZ2	3:D:3244:TRS:H12	2.31	0.66
1:A:114:LYS:HE2	1:A:292:GLU:HG2	1.77	0.66
1:A:162:VAL:HG22	1:A:166:TRP:CD1	2.30	0.66
1:A:214:THR:HB	1:A:366:ILE:HD11	1.77	0.65
1:B:250:LEU:HD23	1:B:343:GLN:CG	2.23	0.65
1:D:303:VAL:HG23	1:D:305:TYR:CE1	2.31	0.65
1:E:200:GLU:CD	1:E:200:GLU:H	1.97	0.65
1:C:138:LYS:O	1:C:142:ARG:HG3	1.95	0.65
1:A:127:SER:O	1:A:131:MET:HG2	1.96	0.65
1:A:214:THR:HG21	1:A:366:ILE:HD11	1.79	0.65
1:A:214:THR:CB	1:A:366:ILE:HD11	2.27	0.65
1:C:250:LEU:CD2	1:C:343:GLN:HG3	2.25	0.65
1:E:398:ARG:HD3	4:E:3343:HOH:O	1.97	0.64
1:A:87:LYS:HG2	1:A:310:ILE:HD13	1.80	0.64
1:D:183:ARG:HG2	1:D:414:GLU:HB3	1.80	0.64
1:F:120:GLY:H	3:F:3249:TRS:H32	1.63	0.64
1:A:392:LEU:HD13	1:A:421:MET:HB2	1.80	0.63
1:C:422:ARG:HG2	4:C:3329:HOH:O	1.98	0.63
1:D:339:TYR:O	1:D:343:GLN:HG2	1.98	0.63
1:F:119:VAL:HG13	3:F:3249:TRS:H31	1.80	0.63
1:A:100:CYS:HA	1:A:103:MET:HE3	1.81	0.63
1:A:383:LYS:HB2	1:A:386:GLU:HG3	1.80	0.63
1:A:356:GLU:HG2	1:A:438:LEU:HD13	1.81	0.63
1:A:49:GLU:O	1:B:92:GLN:HG2	1.98	0.63
1:E:121:THR:OG1	3:E:3246:TRS:H11	1.99	0.63
1:A:192:LYS:O	1:A:196:GLU:HG3	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:190:ASP:OD1	1:C:193:ARG:HD3	1.99	0.62
1:E:221:GLN:HB3	1:E:222:PRO:HD3	1.81	0.62
1:B:31:ARG:NH1	1:B:34:LEU:HD11	2.15	0.62
1:D:415:ALA:HB1	1:D:418:ILE:HD12	1.82	0.62
1:C:121:THR:HA	3:C:3243:TRS:C1	2.30	0.62
1:C:192:LYS:O	1:C:196:GLU:HG3	1.99	0.62
1:E:131:MET:CE	1:F:315:ILE:HG23	2.30	0.62
1:E:10:ARG:HE	1:E:12:GLU:HB3	1.63	0.61
1:F:192:LYS:O	1:F:196:GLU:HG3	1.98	0.61
1:F:390:TYR:HA	1:F:455:GLN:HG3	1.82	0.61
3:E:3246:TRS:O2	3:E:3246:TRS:O1	2.16	0.61
1:B:143:LYS:HE3	1:B:298:GLU:OE1	2.00	0.61
1:E:131:MET:HE3	1:F:315:ILE:HG23	1.83	0.61
1:A:182:MET:HG3	1:A:187:LEU:O	2.01	0.60
1:A:92:GLN:HG2	1:B:49:GLU:O	2.01	0.60
1:B:250:LEU:CD2	1:B:343:GLN:HG3	2.27	0.60
1:B:216:ASN:HD21	1:B:366:ILE:HG22	1.65	0.60
1:E:87:LYS:HG2	1:E:310:ILE:HD12	1.82	0.60
1:A:142:ARG:O	1:A:146:GLU:HG3	2.01	0.60
1:B:221:GLN:HB3	1:B:222:PRO:HD3	1.84	0.60
1:F:72:VAL:HG11	3:F:3240:TRS:H22	1.82	0.60
1:B:305:TYR:HB2	1:B:308:GLY:O	2.01	0.60
1:E:183:ARG:HG2	1:E:414:GLU:HB2	1.82	0.59
1:B:200:GLU:H	1:B:200:GLU:CD	2.05	0.59
1:C:362:PRO:CB	1:C:386:GLU:HG2	2.30	0.59
1:D:162:VAL:HG11	1:D:166:TRP:HB2	1.84	0.59
1:D:362:PRO:CB	1:D:386:GLU:HG2	2.32	0.59
1:D:341:LYS:HE2	1:E:19:GLY:O	2.02	0.59
1:A:250:LEU:CD2	1:A:343:GLN:HG3	2.27	0.59
1:C:114:LYS:NZ	1:C:292:GLU:HG2	2.17	0.59
1:F:183:ARG:HD2	1:F:186:GLN:HE21	1.66	0.59
1:E:142:ARG:O	1:E:146:GLU:HG3	2.02	0.59
1:F:84:TRP:HZ2	3:F:3248:TRS:H32	1.67	0.59
1:F:131:MET:CE	1:F:169:PHE:HB2	2.33	0.59
1:A:250:LEU:HD23	1:A:343:GLN:CG	2.27	0.59
1:E:381:LYS:HD2	1:E:418:ILE:HG23	1.84	0.59
1:A:181:PRO:O	1:A:193:ARG:NH2	2.36	0.59
1:A:87:LYS:HG2	1:A:310:ILE:CD1	2.32	0.59
1:C:135:MET:HE1	1:D:172:TYR:CD1	2.38	0.59
1:A:114:LYS:CD	1:A:114:LYS:H	2.15	0.58
1:E:84:TRP:HZ2	3:E:3246:TRS:H12	1.67	0.58
1:E:339:TYR:O	1:E:343:GLN:HG2	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:101:VAL:HG21	3:A:3251:TRS:H12	1.84	0.58
1:C:127:SER:O	1:C:131:MET:HG2	2.03	0.58
1:D:162:VAL:CG1	1:D:166:TRP:HB2	2.34	0.57
1:B:127:SER:O	1:B:131:MET:HG2	2.04	0.57
1:A:172:TYR:CD1	1:B:135:MET:HE1	2.39	0.57
1:C:121:THR:CA	3:C:3243:TRS:H12	2.35	0.57
1:D:114:LYS:CD	1:D:114:LYS:H	2.15	0.57
1:C:303:VAL:HG23	1:C:305:TYR:CE1	2.40	0.57
1:A:27:ALA:HA	4:A:3382:HOH:O	2.04	0.57
1:A:121:THR:HG1	3:A:3251:TRS:H21	1.70	0.57
1:C:221:GLN:HB3	1:C:222:PRO:HD3	1.87	0.57
1:E:293:GLU:HG3	4:E:3369:HOH:O	2.04	0.57
1:D:356:GLU:HG2	1:D:438:LEU:HD13	1.86	0.57
1:E:181:PRO:O	1:E:193:ARG:NH2	2.32	0.56
1:D:13:LEU:HD12	1:D:13:LEU:N	2.20	0.56
1:E:183:ARG:HE	1:E:414:GLU:HB2	1.69	0.56
1:A:121:THR:OG1	3:A:3251:TRS:H21	2.05	0.56
1:E:254:VAL:HG21	1:E:347:TYR:CE2	2.41	0.56
1:E:22:SER:OG	1:E:23:ILE:N	2.37	0.56
1:B:362:PRO:CB	1:B:386:GLU:HG2	2.36	0.56
1:F:398:ARG:HD3	4:F:3330:HOH:O	2.06	0.56
1:A:92:GLN:NE2	1:A:92:GLN:HA	2.21	0.56
1:E:182:MET:HG2	1:E:187:LEU:O	2.05	0.56
1:B:199:ASP:HB2	1:B:200:GLU:OE2	2.06	0.56
1:B:144:ARG:NH1	1:B:237:ASP:O	2.37	0.56
1:C:411:LEU:O	1:C:416:THR:HA	2.06	0.55
1:B:6:VAL:HA	1:C:257:ASP:HB2	1.89	0.55
1:B:25:THR:O	1:B:29:SER:HB3	2.06	0.55
1:C:114:LYS:NZ	1:C:292:GLU:H	2.04	0.55
1:C:250:LEU:HD23	1:C:343:GLN:CG	2.35	0.54
1:A:395:LEU:HD21	1:A:441:TYR:CZ	2.43	0.54
1:D:293:GLU:HG3	4:D:3371:HOH:O	2.07	0.54
1:C:422:ARG:HG2	1:C:422:ARG:HH11	1.72	0.54
1:B:121:THR:HA	3:B:3242:TRS:C1	2.37	0.54
1:B:124:ILE:HD13	1:B:319:ARG:HD2	1.90	0.54
1:D:162:VAL:HG22	1:D:166:TRP:CD1	2.43	0.54
1:D:13:LEU:N	4:D:3293:HOH:O	2.41	0.54
1:A:183:ARG:HG2	1:A:414:GLU:CB	2.30	0.54
1:D:242:ILE:HD13	1:D:267:VAL:HG13	1.89	0.54
1:D:402:ARG:HD2	1:D:440:ASP:OD1	2.08	0.54
1:D:362:PRO:CG	1:D:388:PRO:HG3	2.37	0.53
1:C:65:GLN:HG3	3:C:3250:TRS:N	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:87:LYS:HG2	1:C:310:ILE:HD12	1.88	0.53
1:C:333:ARG:HH21	1:C:427:ARG:HH22	1.57	0.53
1:F:290:ARG:HD3	4:F:3329:HOH:O	2.08	0.53
1:E:84:TRP:CZ2	3:E:3246:TRS:H12	2.44	0.53
1:A:141:TRP:O	1:A:145:MET:HG2	2.08	0.53
1:F:141:TRP:CZ3	1:F:155:PRO:HB3	2.44	0.53
1:C:298:GLU:CD	1:C:298:GLU:H	2.12	0.53
1:F:121:THR:CB	3:F:3248:TRS:H31	2.39	0.53
1:E:11:SER:O	1:E:22:SER:HB2	2.09	0.53
1:D:228:ASP:HA	1:D:266:ARG:HH21	1.73	0.53
1:F:415:ALA:HB1	1:F:418:ILE:HD12	1.90	0.53
1:A:164:ILE:HD13	1:A:168:LYS:HE3	1.90	0.53
1:E:184:PRO:HA	3:E:3253:TRS:H12	1.91	0.53
1:A:97:ASP:OD2	3:A:3251:TRS:H11	2.09	0.52
1:C:121:THR:CB	3:C:3243:TRS:H12	2.39	0.52
1:B:224:HIS:CD2	1:B:264:LEU:HB3	2.43	0.52
1:C:344:ASN:O	1:C:348:GLN:HG3	2.09	0.52
1:D:362:PRO:HG3	1:D:388:PRO:HG3	1.91	0.52
1:E:10:ARG:HG3	1:E:12:GLU:HG3	1.92	0.52
1:E:344:ASN:O	1:E:348:GLN:HG3	2.10	0.52
1:D:127:SER:O	1:D:131:MET:HG2	2.10	0.52
1:C:216:ASN:HD21	1:C:366:ILE:HG22	1.75	0.52
1:C:242:ILE:HD11	1:C:267:VAL:HG22	1.92	0.52
1:B:121:THR:OG1	3:B:3242:TRS:H12	2.10	0.52
1:E:36:GLU:HG3	1:F:337:GLU:HG2	1.92	0.52
1:C:343:GLN:HA	1:C:343:GLN:OE1	2.09	0.51
1:E:183:ARG:HE	1:E:414:GLU:CB	2.23	0.51
1:F:84:TRP:CZ2	3:F:3248:TRS:H32	2.45	0.51
1:A:162:VAL:CG1	1:A:166:TRP:HB2	2.40	0.51
1:E:312:THR:HG22	3:E:3246:TRS:O3	2.11	0.51
1:E:163:GLN:HG2	4:E:3307:HOH:O	2.10	0.51
1:E:65:GLN:HB3	3:E:3239:TRS:O1	2.11	0.51
1:F:183:ARG:NE	1:F:414:GLU:HG2	2.24	0.51
1:B:122:ASN:HB2	1:B:286:TRP:CZ3	2.46	0.51
1:A:38:ARG:HH21	1:A:40:ASP:HB2	1.76	0.51
3:E:3239:TRS:H21	4:E:3380:HOH:O	2.10	0.51
1:F:141:TRP:CD2	1:F:203:ILE:HG22	2.45	0.51
1:C:281:PRO:HD3	3:C:3250:TRS:O1	2.10	0.51
1:E:415:ALA:HB1	1:E:418:ILE:HD12	1.93	0.51
1:F:97:ASP:OD2	3:F:3248:TRS:O3	2.23	0.50
1:B:344:ASN:O	1:B:348:GLN:HG3	2.11	0.50
1:F:356:GLU:HG2	1:F:438:LEU:CD1	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:3238:TRS:O3	3:D:3238:TRS:O1	2.16	0.50
1:F:120:GLY:N	3:F:3249:TRS:H32	2.26	0.50
1:A:25:THR:O	1:A:29:SER:HB3	2.11	0.50
1:A:224:HIS:CD2	1:A:264:LEU:HB3	2.47	0.50
2:C:1502:PLR:O2P	1:D:318:SER:HB2	2.11	0.50
1:F:245:ALA:HA	1:F:272:ALA:HA	1.93	0.50
1:D:183:ARG:HG2	1:D:414:GLU:CB	2.42	0.50
1:A:400:ARG:CZ	1:B:306:LEU:HD21	2.42	0.50
1:A:38:ARG:HB2	1:A:41:VAL:HG23	1.93	0.50
1:B:192:LYS:O	1:B:196:GLU:HG3	2.12	0.50
1:A:177:LEU:C	1:A:177:LEU:HD13	2.32	0.49
1:E:329:TYR:CZ	1:E:333:ARG:HD3	2.47	0.49
1:B:41:VAL:O	1:B:45:ILE:HG13	2.12	0.49
1:A:38:ARG:HB2	1:A:41:VAL:CG2	2.42	0.49
1:C:139:TRP:CE2	1:C:299:LEU:HD21	2.47	0.49
1:D:395:LEU:HD21	1:D:441:TYR:CZ	2.47	0.49
1:E:171:ARG:NH1	1:F:298:GLU:O	2.44	0.49
1:D:250:LEU:HD12	1:D:375:ILE:HG22	1.94	0.49
1:C:61:ALA:HB2	1:C:407:PRO:HD3	1.94	0.49
1:B:121:THR:HA	3:B:3242:TRS:H12	1.94	0.49
1:E:264:LEU:O	1:E:290:ARG:NH2	2.46	0.49
1:F:129:ALA:HB1	1:F:287:VAL:HB	1.95	0.49
1:B:275:HIS:HA	1:B:280:ALA:O	2.13	0.49
1:A:162:VAL:HG11	1:A:166:TRP:HB2	1.93	0.49
1:F:343:GLN:HA	1:F:343:GLN:OE1	2.13	0.49
1:A:128:GLU:HA	1:A:131:MET:HG3	1.94	0.49
1:E:329:TYR:CE2	1:E:333:ARG:HD3	2.48	0.49
1:C:217:TYR:CD2	1:C:374:GLY:HA2	2.48	0.49
1:B:183:ARG:NE	1:B:414:GLU:OE2	2.46	0.48
1:E:362:PRO:CB	1:E:386:GLU:HG2	2.42	0.48
1:B:72:VAL:HG11	3:B:3237:TRS:H32	1.95	0.48
1:D:124:ILE:HD11	1:D:319:ARG:HD2	1.95	0.48
1:C:333:ARG:HH22	1:C:427:ARG:HH12	1.60	0.48
1:A:344:ASN:O	1:A:348:GLN:HG3	2.13	0.48
1:C:340:THR:O	1:C:344:ASN:HB2	2.13	0.48
1:C:28:GLU:HG2	1:C:31:ARG:HH21	1.79	0.48
1:B:142:ARG:O	1:B:146:GLU:HG3	2.13	0.48
1:E:382:LEU:HD22	1:E:388:PRO:HG2	1.95	0.47
1:D:162:VAL:HG13	1:D:163:GLN:O	2.15	0.47
1:A:122:ASN:HB2	1:A:286:TRP:CZ3	2.49	0.47
1:C:141:TRP:CZ3	1:C:155:PRO:HG3	2.49	0.47
1:A:154:LYS:O	1:A:201:ASN:HB3	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:19:GLY:O	1:F:341:LYS:HE2	2.14	0.47
1:D:319:ARG:HB2	1:D:320:PRO:HD2	1.96	0.47
1:E:183:ARG:CG	1:E:414:GLU:HB2	2.43	0.47
1:D:303:VAL:HG23	1:D:305:TYR:HE1	1.77	0.47
1:E:25:THR:O	1:E:29:SER:HB3	2.14	0.47
1:D:356:GLU:HG2	1:D:438:LEU:CD1	2.44	0.47
1:C:414:GLU:O	1:C:414:GLU:HG2	2.14	0.47
1:A:254:VAL:HG21	1:A:347:TYR:CE2	2.49	0.47
1:B:121:THR:CB	3:B:3242:TRS:H12	2.44	0.47
1:C:114:LYS:HZ2	1:C:292:GLU:CG	2.26	0.47
1:A:163:GLN:HG2	4:A:3293:HOH:O	2.14	0.47
1:B:411:LEU:O	1:B:416:THR:HA	2.15	0.47
1:D:61:ALA:HB2	1:D:407:PRO:HD3	1.96	0.47
1:B:7:THR:HA	1:C:255:ALA:HA	1.95	0.47
1:B:422:ARG:HH11	1:B:422:ARG:HG2	1.80	0.47
1:C:315:ILE:HD13	1:D:315:ILE:HD13	1.96	0.47
1:B:46:ILE:O	1:B:50:LEU:HG	2.14	0.47
1:E:362:PRO:CG	1:E:388:PRO:HG3	2.45	0.47
1:A:402:ARG:HD2	1:A:440:ASP:OD1	2.15	0.47
1:E:306:LEU:HD21	1:F:400:ARG:CZ	2.45	0.47
1:B:269:SER:HB3	1:B:289:TRP:CD1	2.50	0.47
1:A:398:ARG:HD3	4:A:3318:HOH:O	2.15	0.47
1:D:275:HIS:HA	1:D:280:ALA:O	2.14	0.47
1:D:224:HIS:CD2	1:D:264:LEU:HB3	2.50	0.47
1:B:31:ARG:HH11	1:B:34:LEU:HD11	1.80	0.47
1:C:41:VAL:O	1:C:45:ILE:HG13	2.14	0.47
1:B:182:MET:HG3	1:B:187:LEU:O	2.15	0.47
1:A:38:ARG:HB3	1:A:38:ARG:HE	1.52	0.46
1:D:242:ILE:CD1	1:D:267:VAL:HG22	2.42	0.46
1:E:356:GLU:HG2	1:E:438:LEU:HD13	1.97	0.46
1:E:337:GLU:HB2	4:F:3399:HOH:O	2.15	0.46
1:D:239:ASP:OD2	1:D:268:LYS:NZ	2.47	0.46
1:A:188:PHE:HZ	1:A:216:ASN:HD22	1.64	0.46
1:C:143:LYS:HE3	1:C:298:GLU:OE1	2.16	0.46
1:C:224:HIS:CD2	1:C:266:ARG:HB2	2.51	0.46
1:F:121:THR:HA	3:F:3248:TRS:H31	1.97	0.46
1:A:356:GLU:HG2	1:A:438:LEU:CD1	2.46	0.46
1:D:163:GLN:HG2	4:D:3356:HOH:O	2.16	0.46
1:A:109:HIS:HD2	1:A:261:ASP:OD2	1.98	0.46
1:D:186:GLN:O	1:D:186:GLN:HG3	2.15	0.46
1:B:52:LEU:HB3	3:C:3252:TRS:H32	1.98	0.46
1:D:414:GLU:C	1:D:416:THR:H	2.19	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:195:ILE:HD11	1:A:230:PHE:HB2	1.98	0.46
1:D:181:PRO:O	1:D:193:ARG:NH2	2.45	0.46
1:A:343:GLN:HA	1:A:343:GLN:OE1	2.15	0.46
1:F:23:ILE:HG21	1:F:37:MET:CE	2.46	0.46
1:D:381:LYS:HE2	4:D:3386:HOH:O	2.16	0.46
1:F:344:ASN:O	1:F:348:GLN:HG3	2.17	0.45
1:A:91:PRO:HB2	3:C:3252:TRS:C1	2.39	0.45
1:E:182:MET:CE	1:E:187:LEU:HB3	2.45	0.45
1:B:16:SER:O	1:C:427:ARG:HD2	2.16	0.45
1:B:180:ILE:HD12	1:B:180:ILE:N	2.31	0.45
1:E:183:ARG:HE	1:E:414:GLU:CG	2.29	0.45
1:C:245:ALA:HA	1:C:272:ALA:HA	1.97	0.45
1:B:124:ILE:HD11	1:B:319:ARG:HD2	1.97	0.45
1:F:216:ASN:HD21	1:F:366:ILE:HG22	1.82	0.45
1:E:122:ASN:HB2	1:E:286:TRP:CZ3	2.51	0.45
1:B:245:ALA:HA	1:B:272:ALA:HA	1.99	0.45
1:C:63:PHE:HA	1:C:424:MET:HE2	1.98	0.45
1:F:72:VAL:HG11	3:F:3240:TRS:H12	1.99	0.45
1:E:131:MET:HE2	1:F:315:ILE:HG23	1.99	0.45
1:E:217:TYR:CD2	1:E:374:GLY:HA2	2.51	0.45
1:C:13:LEU:N	4:C:3318:HOH:O	2.50	0.45
1:B:157:LEU:HD22	1:B:204:GLY:O	2.17	0.45
1:A:139:TRP:O	1:A:143:LYS:HG3	2.16	0.45
1:F:25:THR:O	1:F:29:SER:HB3	2.17	0.45
1:F:182:MET:HG3	1:F:187:LEU:O	2.16	0.45
1:B:163:GLN:HG2	4:B:3339:HOH:O	2.16	0.45
1:F:46:ILE:O	1:F:50:LEU:HG	2.16	0.45
1:D:245:ALA:HA	1:D:272:ALA:HA	1.98	0.45
1:A:89:GLU:C	1:A:91:PRO:HD3	2.37	0.45
1:D:390:TYR:CA	1:D:455:GLN:HG3	2.45	0.45
1:F:121:THR:HB	3:F:3249:TRS:O2	2.17	0.45
1:F:98:LEU:HD23	3:F:3248:TRS:O1	2.17	0.45
1:E:97:ASP:OD2	3:E:3246:TRS:O1	2.33	0.45
1:D:163:GLN:NE2	1:D:164:ILE:HG22	2.31	0.45
1:B:301:PHE:O	1:B:312:THR:HG22	2.17	0.45
1:C:312:THR:HG22	3:C:3243:TRS:O2	2.16	0.45
1:B:119:VAL:HG22	1:B:292:GLU:OE2	2.17	0.45
1:C:65:GLN:HG3	3:C:3250:TRS:HN1	1.80	0.44
1:F:221:GLN:CB	1:F:222:PRO:HD3	2.45	0.44
1:C:122:ASN:HB2	1:C:286:TRP:CZ3	2.53	0.44
1:D:83:ASN:OD1	1:D:85:ILE:HG22	2.17	0.44
1:E:154:LYS:HB3	1:E:154:LYS:HE2	1.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:124:ILE:HD13	1:E:124:ILE:HA	1.87	0.44
1:A:315:ILE:HD13	1:B:315:ILE:HD13	1.98	0.44
1:E:62:THR:HA	1:E:466:THR:OXT	2.18	0.44
1:E:183:ARG:HE	1:E:414:GLU:HG2	1.82	0.44
1:A:156:ASN:OD1	1:A:202:THR:HA	2.16	0.44
1:F:30:LYS:C	1:F:31:ARG:HD2	2.37	0.44
1:E:61:ALA:HB2	1:E:407:PRO:HD3	2.00	0.44
1:A:186:GLN:O	1:A:186:GLN:HG3	2.17	0.44
1:F:463:PHE:CE2	1:F:466:THR:HG22	2.52	0.44
1:A:228:ASP:HA	1:A:266:ARG:HH21	1.82	0.44
1:A:59:ASN:HA	1:A:405:GLN:HB3	1.98	0.44
1:D:65:GLN:HB3	3:D:3238:TRS:HN1	1.81	0.44
1:E:395:LEU:HD21	1:E:441:TYR:CZ	2.52	0.44
1:A:114:LYS:CE	1:A:292:GLU:HG2	2.47	0.44
1:D:382:LEU:HD22	1:D:388:PRO:HG2	2.00	0.44
1:F:398:ARG:HD2	1:F:398:ARG:N	2.31	0.44
1:A:400:ARG:HA	1:A:404:TRP:O	2.17	0.44
1:E:400:ARG:HA	1:E:404:TRP:O	2.18	0.44
1:F:59:ASN:HA	1:F:405:GLN:HB3	1.99	0.44
1:A:101:VAL:CG2	3:A:3251:TRS:H12	2.47	0.44
1:F:61:ALA:HB2	1:F:407:PRO:HD3	2.00	0.44
1:F:163:GLN:HG2	4:F:3308:HOH:O	2.18	0.44
1:A:98:LEU:CD2	3:A:3251:TRS:O3	2.65	0.44
1:A:453:LYS:NZ	4:A:3435:HOH:O	2.51	0.44
1:B:264:LEU:O	1:B:290:ARG:NH2	2.51	0.43
1:F:24:SER:HB3	1:F:27:ALA:HB3	2.00	0.43
1:E:275:HIS:HA	1:E:280:ALA:O	2.17	0.43
1:C:58:GLN:HE22	3:C:3252:TRS:H31	1.83	0.43
1:A:161:PRO:HB3	1:A:182:MET:HE3	2.00	0.43
1:C:454:LEU:HA	1:C:457:ILE:HD12	2.00	0.43
1:D:459:GLN:HB3	1:D:459:GLN:HE21	1.49	0.43
1:E:410:THR:HA	1:E:418:ILE:O	2.18	0.43
1:A:162:VAL:HG13	1:A:163:GLN:O	2.18	0.43
1:A:217:TYR:CD2	1:A:374:GLY:HA2	2.53	0.43
1:A:190:ASP:HA	4:A:3322:HOH:O	2.18	0.43
1:F:269:SER:HB3	1:F:289:TRP:CD1	2.53	0.43
1:A:319:ARG:HB2	1:A:320:PRO:HD2	2.00	0.43
1:F:121:THR:CA	3:F:3248:TRS:H31	2.48	0.43
1:C:329:TYR:CE2	1:C:333:ARG:HD3	2.54	0.43
1:C:400:ARG:HA	1:C:404:TRP:O	2.19	0.43
1:D:160:GLY:O	1:D:179:GLU:HG3	2.18	0.43
1:F:362:PRO:HB2	1:F:386:GLU:HG2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:GLU:HG2	1:B:337:GLU:OE2	2.19	0.43
1:D:410:THR:HG22	1:D:419:VAL:HG22	2.00	0.43
1:B:343:GLN:OE1	1:B:343:GLN:HA	2.19	0.43
1:B:242:ILE:CD1	1:B:267:VAL:HG22	2.49	0.43
1:B:432:ASP:HA	1:C:26:ILE:HD12	2.01	0.43
1:C:183:ARG:HH11	1:C:183:ARG:HG2	1.84	0.42
1:A:164:ILE:HD12	1:A:164:ILE:C	2.38	0.42
1:A:162:VAL:CG2	1:A:166:TRP:CD1	3.01	0.42
1:E:114:LYS:HE2	4:E:3369:HOH:O	2.18	0.42
1:E:185:GLY:H	3:E:3253:TRS:C1	2.32	0.42
1:D:255:ALA:N	1:D:256:PRO:HD3	2.34	0.42
1:D:242:ILE:HD13	1:D:267:VAL:CG1	2.50	0.42
1:A:262:PHE:O	1:A:290:ARG:NH2	2.51	0.42
1:C:465:HIS:O	1:C:466:THR:HB	2.19	0.42
1:A:417:ASP:HB2	4:A:3419:HOH:O	2.18	0.42
3:A:3236:TRS:H12	4:A:3437:HOH:O	2.18	0.42
1:A:216:ASN:HD21	1:A:366:ILE:HG13	1.83	0.42
1:A:162:VAL:HG22	1:A:166:TRP:HD1	1.81	0.42
1:E:460:GLN:HG2	1:F:306:LEU:O	2.18	0.42
1:D:252:PRO:HG3	4:D:3282:HOH:O	2.18	0.42
1:D:254:VAL:HG21	1:D:347:TYR:CE2	2.54	0.42
1:E:343:GLN:OE1	1:E:343:GLN:HA	2.19	0.42
1:D:219:PHE:HA	1:D:220:PRO:HD3	1.85	0.42
1:D:217:TYR:CD2	1:D:374:GLY:HA2	2.54	0.42
1:E:10:ARG:HG3	1:E:12:GLU:CG	2.50	0.42
1:D:242:ILE:HD12	1:D:242:ILE:N	2.34	0.42
1:E:154:LYS:O	1:E:201:ASN:HB3	2.19	0.42
1:D:177:LEU:CD1	1:D:179:GLU:HB2	2.49	0.42
1:F:314:ALA:HB2	4:F:3340:HOH:O	2.20	0.42
1:B:299:LEU:HB3	1:B:313:PHE:CE1	2.54	0.42
1:E:261:ASP:HB2	1:E:262:PHE:H	1.59	0.42
1:E:12:GLU:HB2	1:E:13:LEU:H	1.65	0.42
1:E:121:THR:HA	3:E:3246:TRS:H11	2.00	0.42
1:A:264:LEU:O	1:A:290:ARG:NH2	2.52	0.42
1:A:303:VAL:HB	1:B:465:HIS:CD2	2.55	0.42
1:B:59:ASN:HA	1:B:405:GLN:HB3	2.02	0.42
1:A:128:GLU:O	1:A:132:LEU:HG	2.19	0.42
1:B:135:MET:HE2	1:B:135:MET:HB3	1.83	0.42
1:D:264:LEU:O	1:D:290:ARG:NH2	2.53	0.42
1:A:390:TYR:N	1:A:455:GLN:NE2	2.67	0.42
1:E:303:VAL:HG23	1:E:305:TYR:CE2	2.55	0.42
1:A:129:ALA:HB1	1:A:287:VAL:HB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:23:ILE:HG21	1:D:37:MET:CE	2.49	0.42
1:B:89:GLU:C	1:B:91:PRO:HD3	2.40	0.42
1:F:250:LEU:HD23	1:F:343:GLN:CG	2.29	0.42
1:D:451:HIS:N	1:D:452:PRO:HD3	2.35	0.42
1:A:245:ALA:HA	1:A:272:ALA:HA	2.02	0.42
1:C:199:ASP:OD1	1:C:201:ASN:N	2.43	0.42
1:F:72:VAL:CG2	3:F:3240:TRS:H12	2.38	0.42
1:B:319:ARG:HB2	1:B:320:PRO:CD	2.50	0.42
1:E:200:GLU:HG3	1:E:236:ILE:HD11	2.02	0.42
1:D:465:HIS:O	1:D:466:THR:HB	2.20	0.42
1:B:427:ARG:HH21	3:B:3237:TRS:H21	1.84	0.41
1:E:157:LEU:HD12	1:E:204:GLY:O	2.20	0.41
1:A:275:HIS:HA	1:A:280:ALA:O	2.20	0.41
1:B:117:GLN:HB2	4:B:3389:HOH:O	2.20	0.41
1:D:98:LEU:HD23	3:D:3244:TRS:O3	2.21	0.41
1:B:465:HIS:O	1:B:466:THR:HB	2.20	0.41
1:B:63:PHE:HA	1:B:424:MET:HE2	2.01	0.41
1:F:395:LEU:HD21	1:F:441:TYR:CZ	2.55	0.41
1:E:388:PRO:HB2	1:E:390:TYR:CE2	2.55	0.41
1:B:6:VAL:CA	1:C:257:ASP:HB2	2.49	0.41
1:B:126:SER:HB2	2:B:1501:PLR:O4P	2.20	0.41
1:C:67:TRP:O	3:C:3250:TRS:H32	2.21	0.41
1:E:10:ARG:C	1:E:12:GLU:H	2.23	0.41
1:A:142:ARG:O	1:A:145:MET:HB2	2.21	0.41
1:A:159:CYS:SG	1:A:177:LEU:HD11	2.60	0.41
1:F:319:ARG:HB2	1:F:320:PRO:HD2	2.01	0.41
1:F:180:ILE:HD12	1:F:180:ILE:N	2.35	0.41
1:C:46:ILE:O	1:C:50:LEU:HG	2.20	0.41
1:E:362:PRO:HG3	1:E:388:PRO:HG3	2.01	0.41
1:B:153:ASP:OD2	1:B:154:LYS:HG3	2.21	0.41
1:B:451:HIS:N	1:B:452:PRO:HD3	2.35	0.41
1:D:344:ASN:HD22	1:D:344:ASN:HA	1.66	0.41
1:C:275:HIS:HA	1:C:280:ALA:O	2.20	0.41
1:E:37:MET:HE1	1:F:332:LEU:HD22	2.03	0.41
1:B:400:ARG:HA	1:B:404:TRP:O	2.21	0.41
1:C:183:ARG:HH12	1:C:414:GLU:HB2	1.86	0.41
1:A:98:LEU:HD21	3:A:3251:TRS:O3	2.21	0.41
1:E:114:LYS:NZ	1:E:292:GLU:HG2	2.34	0.41
1:B:113:PRO:C	1:B:115:ASN:H	2.23	0.41
1:C:371:PRO:HD2	4:C:3367:HOH:O	2.20	0.41
1:E:114:LYS:HG3	1:E:114:LYS:H	1.61	0.41
1:D:344:ASN:O	1:D:348:GLN:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:157:LEU:HD22	1:A:204:GLY:O	2.21	0.41
1:F:451:HIS:N	1:F:452:PRO:HD3	2.36	0.41
1:B:352:TYR:OH	1:B:435:GLU:OE2	2.26	0.41
1:E:255:ALA:N	1:E:256:PRO:HD3	2.36	0.41
1:A:293:GLU:H	1:A:293:GLU:CD	2.23	0.41
1:A:131:MET:CE	1:A:169:PHE:HB2	2.51	0.41
1:D:141:TRP:CZ3	1:D:155:PRO:HB3	2.56	0.41
1:B:139:TRP:HB3	1:B:296:PRO:HG2	2.01	0.41
1:A:187:LEU:HD12	1:A:366:ILE:HD12	2.02	0.41
1:F:186:GLN:O	1:F:186:GLN:HG3	2.21	0.41
1:B:98:LEU:HD23	3:B:3242:TRS:O3	2.21	0.41
1:E:185:GLY:N	3:E:3253:TRS:O1	2.49	0.41
1:A:400:ARG:NE	1:B:306:LEU:HD21	2.36	0.41
1:C:228:ASP:HA	1:C:266:ARG:HH21	1.85	0.41
1:C:177:LEU:HD11	1:C:179:GLU:HB2	2.03	0.41
1:D:182:MET:HG2	1:D:187:LEU:HD22	2.03	0.41
1:C:218:GLU:O	1:C:220:PRO:HD3	2.21	0.41
1:C:395:LEU:HD21	1:C:441:TYR:CZ	2.56	0.41
1:A:112:ALA:HA	1:A:113:PRO:HD3	1.97	0.41
1:C:58:GLN:NE2	3:C:3252:TRS:H31	2.35	0.41
1:A:182:MET:HG2	1:A:187:LEU:HD22	2.03	0.41
1:C:114:LYS:HE2	4:C:3389:HOH:O	2.21	0.41
1:E:182:MET:HE2	1:E:187:LEU:HD22	2.03	0.41
1:C:417:ASP:HB3	4:C:3311:HOH:O	2.21	0.41
1:B:61:ALA:HB2	1:B:407:PRO:HD3	2.02	0.41
1:F:275:HIS:NE2	2:F:1505:PLR:O1P	2.48	0.41
1:A:72:VAL:HG11	3:A:3236:TRS:H22	2.03	0.40
3:D:3244:TRS:H21	3:D:3245:TRS:O3	2.20	0.40
1:C:219:PHE:HA	1:C:220:PRO:HD3	1.87	0.40
1:C:112:ALA:HA	1:C:113:PRO:HD3	1.93	0.40
1:E:306:LEU:HD21	1:F:400:ARG:NE	2.36	0.40
1:E:63:PHE:CD1	1:E:63:PHE:N	2.89	0.40
1:E:183:ARG:NH2	1:E:414:GLU:HG2	2.29	0.40
1:E:286:TRP:HZ2	1:E:327:GLN:HG2	1.86	0.40
1:A:154:LYS:HE2	1:A:154:LYS:HB3	1.85	0.40
1:B:242:ILE:HD11	1:B:267:VAL:HG22	2.02	0.40
1:B:141:TRP:CZ3	1:B:155:PRO:HG3	2.57	0.40
1:D:286:TRP:HZ2	1:D:327:GLN:HG2	1.85	0.40
1:F:400:ARG:HA	1:F:404:TRP:O	2.21	0.40
1:B:157:LEU:HD13	1:B:157:LEU:C	2.42	0.40
1:C:370:ARG:HA	1:C:371:PRO:HD3	1.88	0.40

There are no symmetry-related clashes.

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	453/466 (97%)	436 (96%)	15 (3%)	2 (0%)	43	52
1	B	461/466 (99%)	446 (97%)	14 (3%)	1 (0%)	56	68
1	C	452/466 (97%)	436 (96%)	14 (3%)	2 (0%)	43	52
1	D	452/466 (97%)	437 (97%)	15 (3%)	0	100	100
1	E	461/466 (99%)	437 (95%)	20 (4%)	4 (1%)	25	26
1	F	452/466 (97%)	440 (97%)	12 (3%)	0	100	100
All	All	2731/2796 (98%)	2632 (96%)	90 (3%)	9 (0%)	50	60

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	27	ALA
1	E	12	GLU
1	A	385	GLY
1	B	116	GLY
1	C	116	GLY
1	E	13	LEU
1	E	22	SER
1	A	387	ASP
1	E	23	ILE

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	379/390 (97%)	371 (98%)	8 (2%)	66	83
1	B	387/390 (99%)	377 (97%)	10 (3%)	59	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	378/390 (97%)	371 (98%)	7 (2%)	69	85
1	D	378/390 (97%)	372 (98%)	6 (2%)	75	88
1	E	387/390 (99%)	380 (98%)	7 (2%)	71	86
1	F	378/390 (97%)	371 (98%)	7 (2%)	69	85
All	All	2287/2340 (98%)	2242 (98%)	45 (2%)	68	84

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	LYS
1	A	162	VAL
1	A	200	GLU
1	A	268	LYS
1	A	293	GLU
1	A	343	GLN
1	A	366	ILE
1	A	414	GLU
1	B	10	ARG
1	B	124	ILE
1	B	139	TRP
1	B	150	LYS
1	B	153	ASP
1	B	195	ILE
1	B	268	LYS
1	B	343	GLN
1	B	355	ASP
1	B	414	GLU
1	C	268	LYS
1	C	304	ASP
1	C	343	GLN
1	C	344	ASN
1	C	427	ARG
1	C	437	LEU
1	C	459	GLN
1	D	114	LYS
1	D	162	VAL
1	D	268	LYS
1	D	304	ASP
1	D	398	ARG
1	D	459	GLN
1	E	8	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	12	GLU
1	E	21	LYS
1	E	31	ARG
1	E	126	SER
1	E	142	ARG
1	E	268	LYS
1	F	131	MET
1	F	221	GLN
1	F	304	ASP
1	F	343	GLN
1	F	386	GLU
1	F	414	GLU
1	F	437	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	92	GLN
1	A	109	HIS
1	A	186	GLN
1	A	216	ASN
1	A	297	GLN
1	A	309	GLN
1	A	344	ASN
1	A	405	GLN
1	A	459	GLN
1	B	5	GLN
1	B	109	HIS
1	B	216	ASN
1	B	309	GLN
1	B	459	GLN
1	C	58	GLN
1	C	109	HIS
1	C	186	GLN
1	C	216	ASN
1	C	309	GLN
1	C	459	GLN
1	D	167	HIS
1	D	309	GLN
1	D	344	ASN
1	D	459	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	5	GLN
1	E	221	GLN
1	E	309	GLN
1	E	344	ASN
1	F	58	GLN
1	F	186	GLN
1	F	216	ASN
1	F	309	GLN
1	F	344	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

24 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	PLR	A	1500	-	15,15,15	0.74	0	22,22,22	1.38	5 (22%)
3	TRS	A	3236	-	7,7,7	1.04	1 (14%)	9,9,9	0.45	0
3	TRS	A	3241	-	7,7,7	0.97	1 (14%)	9,9,9	0.58	0
3	TRS	A	3251	-	7,7,7	0.89	1 (14%)	9,9,9	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLR	B	1501	-	15,15,15	0.96	1 (6%)	22,22,22	1.45	6 (27%)
3	TRS	B	3237	-	7,7,7	1.02	1 (14%)	9,9,9	0.58	0
3	TRS	B	3242	-	7,7,7	0.97	1 (14%)	9,9,9	0.56	0
2	PLR	C	1502	-	15,15,15	1.05	1 (6%)	22,22,22	1.40	6 (27%)
3	TRS	C	3243	-	7,7,7	0.94	1 (14%)	9,9,9	0.65	0
3	TRS	C	3250	-	7,7,7	1.03	1 (14%)	9,9,9	0.38	0
3	TRS	C	3252	-	7,7,7	0.93	1 (14%)	9,9,9	0.63	0
2	PLR	D	1503	-	15,15,15	1.03	1 (6%)	22,22,22	1.44	6 (27%)
3	TRS	D	3238	-	7,7,7	1.04	1 (14%)	9,9,9	0.53	0
3	TRS	D	3244	-	7,7,7	1.01	1 (14%)	9,9,9	0.58	0
3	TRS	D	3245	-	7,7,7	0.91	1 (14%)	9,9,9	0.71	0
2	PLR	E	1504	-	15,15,15	1.00	1 (6%)	22,22,22	1.42	6 (27%)
3	TRS	E	3239	-	7,7,7	1.05	1 (14%)	9,9,9	0.37	0
3	TRS	E	3246	-	7,7,7	1.13	1 (14%)	9,9,9	0.48	0
3	TRS	E	3247	-	7,7,7	0.93	1 (14%)	9,9,9	0.78	0
3	TRS	E	3253	-	7,7,7	0.96	1 (14%)	9,9,9	0.54	0
2	PLR	F	1505	-	15,15,15	1.04	1 (6%)	22,22,22	1.43	6 (27%)
3	TRS	F	3240	-	7,7,7	0.98	1 (14%)	9,9,9	0.67	0
3	TRS	F	3248	-	7,7,7	0.92	1 (14%)	9,9,9	0.50	0
3	TRS	F	3249	-	7,7,7	1.04	1 (14%)	9,9,9	0.53	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	PLR	A	1500	-	-	0/6/6/6	0/1/1/1
3	TRS	A	3236	-	-	0/9/9/9	0/0/0/0
3	TRS	A	3241	-	-	0/9/9/9	0/0/0/0
3	TRS	A	3251	-	-	0/9/9/9	0/0/0/0
2	PLR	B	1501	-	-	0/6/6/6	0/1/1/1
3	TRS	B	3237	-	-	0/9/9/9	0/0/0/0
3	TRS	B	3242	-	-	0/9/9/9	0/0/0/0
2	PLR	C	1502	-	-	0/6/6/6	0/1/1/1
3	TRS	C	3243	-	-	0/9/9/9	0/0/0/0
3	TRS	C	3250	-	-	0/9/9/9	0/0/0/0
3	TRS	C	3252	-	-	0/9/9/9	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLR	D	1503	-	-	0/6/6/6	0/1/1/1
3	TRS	D	3238	-	-	0/9/9/9	0/0/0/0
3	TRS	D	3244	-	-	0/9/9/9	0/0/0/0
3	TRS	D	3245	-	-	0/9/9/9	0/0/0/0
2	PLR	E	1504	-	-	0/6/6/6	0/1/1/1
3	TRS	E	3239	-	-	0/9/9/9	0/0/0/0
3	TRS	E	3246	-	-	0/9/9/9	0/0/0/0
3	TRS	E	3247	-	-	0/9/9/9	0/0/0/0
3	TRS	E	3253	-	-	0/9/9/9	0/0/0/0
2	PLR	F	1505	-	-	0/6/6/6	0/1/1/1
3	TRS	F	3240	-	-	0/9/9/9	0/0/0/0
3	TRS	F	3248	-	-	0/9/9/9	0/0/0/0
3	TRS	F	3249	-	-	0/9/9/9	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1505	PLR	C3-C2	2.91	1.42	1.40
2	C	1502	PLR	C3-C2	2.90	1.42	1.40
2	E	1504	PLR	C3-C2	2.76	1.42	1.40
2	D	1503	PLR	C3-C2	2.67	1.42	1.40
3	A	3236	TRS	C-N	-2.48	1.47	1.50
3	E	3246	TRS	C-N	-2.48	1.47	1.50
3	D	3244	TRS	C-N	-2.44	1.47	1.50
3	E	3239	TRS	C-N	-2.42	1.47	1.50
3	F	3249	TRS	C-N	-2.41	1.47	1.50
3	F	3240	TRS	C-N	-2.40	1.47	1.50
3	E	3247	TRS	C-N	-2.36	1.47	1.50
3	B	3237	TRS	C-N	-2.34	1.47	1.50
3	C	3250	TRS	C-N	-2.32	1.47	1.50
3	D	3238	TRS	C-N	-2.32	1.47	1.50
3	A	3241	TRS	C-N	-2.27	1.47	1.50
3	C	3243	TRS	C-N	-2.27	1.47	1.50
3	A	3251	TRS	C-N	-2.24	1.47	1.50
3	C	3252	TRS	C-N	-2.22	1.47	1.50
2	B	1501	PLR	C5-C4	2.22	1.43	1.40
3	B	3242	TRS	C-N	-2.20	1.47	1.50
3	D	3245	TRS	C-N	-2.20	1.47	1.50
3	E	3253	TRS	C-N	-2.19	1.47	1.50
3	F	3248	TRS	C-N	-2.18	1.47	1.50

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1501	PLR	C4A-C4-C5	3.30	124.00	120.79
2	F	1505	PLR	C4A-C4-C5	3.15	123.86	120.79
2	D	1503	PLR	C4A-C4-C5	3.04	123.75	120.79
2	C	1502	PLR	C4A-C4-C5	3.03	123.74	120.79
2	A	1500	PLR	C4A-C4-C5	3.01	123.72	120.79
2	E	1504	PLR	C4A-C4-C5	2.87	123.58	120.79
2	E	1504	PLR	O3P-P-O1P	2.53	118.70	110.44
2	A	1500	PLR	O3P-P-O1P	2.52	118.68	110.44
2	D	1503	PLR	O3P-P-O1P	2.47	118.52	110.44
2	F	1505	PLR	O3P-P-O1P	2.47	118.50	110.44
2	B	1501	PLR	O3P-P-O1P	2.45	118.44	110.44
2	E	1504	PLR	C2A-C2-C3	2.36	123.89	121.02
2	D	1503	PLR	C3-C2-N1	-2.34	117.45	120.66
2	E	1504	PLR	C3-C2-N1	-2.32	117.47	120.66
2	C	1502	PLR	O3P-P-O1P	2.32	118.02	110.44
2	F	1505	PLR	C3-C2-N1	-2.31	117.50	120.66
2	C	1502	PLR	C2A-C2-C3	2.29	123.80	121.02
2	D	1503	PLR	C2A-C2-C3	2.29	123.80	121.02
2	B	1501	PLR	C3-C2-N1	-2.27	117.55	120.66
2	D	1503	PLR	C6-N1-C2	2.27	124.14	119.28
2	C	1502	PLR	C3-C2-N1	-2.25	117.57	120.66
2	F	1505	PLR	C2A-C2-C3	2.25	123.75	121.02
2	A	1500	PLR	C3-C2-N1	-2.23	117.60	120.66
2	B	1501	PLR	C6-N1-C2	2.23	124.06	119.28
2	E	1504	PLR	O3-C3-C2	2.18	121.49	117.61
2	F	1505	PLR	O3-C3-C2	2.18	121.48	117.61
2	C	1502	PLR	O3-C3-C2	2.17	121.46	117.61
2	A	1500	PLR	C6-N1-C2	2.16	123.92	119.28
2	C	1502	PLR	C6-N1-C2	2.16	123.91	119.28
2	D	1503	PLR	O3-C3-C2	2.16	121.44	117.61
2	F	1505	PLR	C6-N1-C2	2.14	123.87	119.28
2	E	1504	PLR	C6-N1-C2	2.13	123.84	119.28
2	B	1501	PLR	O3-C3-C2	2.06	121.27	117.61
2	B	1501	PLR	C2A-C2-C3	2.05	123.51	121.02
2	A	1500	PLR	O3-C3-C2	2.02	121.20	117.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	455/466 (97%)	0.05	18 (3%)	36	47	16, 26, 46, 58	0
1	B	463/466 (99%)	0.03	25 (5%)	25	34	16, 27, 47, 56	0
1	C	454/466 (97%)	-0.01	16 (3%)	42	52	13, 25, 47, 59	0
1	D	454/466 (97%)	0.01	23 (5%)	27	37	16, 26, 45, 53	0
1	E	463/466 (99%)	-0.00	24 (5%)	26	36	14, 24, 51, 64	0
1	F	454/466 (97%)	-0.01	20 (4%)	33	43	14, 25, 45, 55	0
All	All	2743/2796 (98%)	0.01	126 (4%)	31	41	13, 26, 47, 64	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	115	ASN	6.8
1	E	12	GLU	6.6
1	F	115	ASN	6.2
1	A	115	ASN	5.8
1	D	115	ASN	5.6
1	A	116	GLY	5.4
1	E	13	LEU	5.1
1	F	385	GLY	4.9
1	E	115	ASN	4.9
1	B	115	ASN	4.9
1	D	116	GLY	4.9
1	B	114	LYS	4.5
1	B	308	GLY	4.4
1	D	13	LEU	4.3
1	A	308	GLY	4.2
1	C	413	GLY	4.1
1	D	147	ALA	3.9
1	D	414	GLU	3.9
1	A	28	GLU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	28	GLU	3.7
1	D	417	ASP	3.6
1	E	28	GLU	3.6
1	C	31	ARG	3.5
1	B	309	GLN	3.5
1	B	112	ALA	3.5
1	A	12	GLU	3.5
1	B	147	ALA	3.5
1	E	7	THR	3.4
1	D	385	GLY	3.4
1	E	310	ILE	3.4
1	A	386	GLU	3.4
1	C	414	GLU	3.3
1	C	415	ALA	3.3
1	C	13	LEU	3.3
1	E	413	GLY	3.3
1	D	459	GLN	3.2
1	E	116	GLY	3.2
1	D	114	LYS	3.2
1	B	414	GLU	3.2
1	B	116	GLY	3.2
1	F	28	GLU	3.1
1	A	27	ALA	3.1
1	C	114	LYS	3.0
1	E	308	GLY	3.0
1	B	416	THR	3.0
1	D	113	PRO	3.0
1	A	114	LYS	3.0
1	D	27	ALA	2.9
1	F	417	ASP	2.9
1	A	387	ASP	2.9
1	F	459	GLN	2.9
1	F	147	ALA	2.8
1	C	116	GLY	2.8
1	D	185	GLY	2.7
1	C	112	ALA	2.7
1	B	303	VAL	2.7
1	C	28	GLU	2.7
1	E	11	SER	2.7
1	F	114	LYS	2.7
1	C	385	GLY	2.7
1	D	305	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	384	ASP	2.6
1	D	149	GLY	2.6
1	D	308	GLY	2.6
1	F	307	GLY	2.6
1	A	186	GLN	2.6
1	F	386	GLU	2.6
1	B	384	ASP	2.5
1	E	309	GLN	2.5
1	D	28	GLU	2.5
1	A	307	GLY	2.5
1	A	385	GLY	2.5
1	E	385	GLY	2.5
1	B	113	PRO	2.5
1	A	30	LYS	2.5
1	A	154	LYS	2.5
1	E	114	LYS	2.5
1	F	13	LEU	2.5
1	E	22	SER	2.5
1	D	257	ASP	2.5
1	B	31	ARG	2.5
1	B	417	ASP	2.4
1	A	414	GLU	2.4
1	A	34	LEU	2.4
1	D	293	GLU	2.4
1	E	306	LEU	2.4
1	E	8	ASP	2.4
1	C	149	GLY	2.3
1	E	415	ALA	2.3
1	B	385	GLY	2.3
1	E	19	GLY	2.3
1	A	13	LEU	2.3
1	F	116	GLY	2.3
1	B	26	ILE	2.3
1	B	143	LYS	2.3
1	E	23	ILE	2.3
1	F	310	ILE	2.3
1	B	297	GLN	2.2
1	B	293	GLU	2.2
1	E	414	GLU	2.2
1	B	257	ASP	2.2
1	F	113	PRO	2.2
1	E	416	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	144	ARG	2.1
1	F	27	ALA	2.1
1	D	183	ARG	2.1
1	F	149	GLY	2.1
1	F	414	GLU	2.1
1	B	310	ILE	2.1
1	B	11	SER	2.1
1	B	153	ASP	2.1
1	C	183	ARG	2.1
1	F	297	GLN	2.1
1	E	305	TYR	2.1
1	D	232	ALA	2.1
1	F	21	LYS	2.1
1	C	307	GLY	2.1
1	A	183	ARG	2.1
1	E	10	ARG	2.1
1	F	183	ARG	2.1
1	C	416	THR	2.1
1	B	148	ALA	2.1
1	E	303	VAL	2.0
1	D	384	ASP	2.0
1	D	386	GLU	2.0
1	D	112	ALA	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 carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	TRS	C	3250	8/8	0.34	12.45	55,56,57,57	0
3	TRS	C	3252	8/8	0.38	10.17	54,54,54,55	0
3	TRS	A	3236	8/8	0.28	10.17	64,64,65,65	0
3	TRS	E	3239	8/8	0.28	9.47	47,48,49,49	0
3	TRS	D	3245	8/8	0.31	8.92	65,65,65,66	0
3	TRS	C	3243	8/8	0.27	8.87	58,60,60,60	0
3	TRS	B	3237	8/8	0.29	8.49	73,73,74,74	0
3	TRS	F	3240	8/8	0.28	7.75	60,61,61,61	0
3	TRS	A	3251	8/8	0.30	4.91	48,49,50,51	0
3	TRS	D	3244	8/8	0.26	4.87	58,58,59,59	0
3	TRS	D	3238	8/8	0.25	4.64	54,55,55,56	0
3	TRS	E	3246	8/8	0.20	4.25	48,51,51,53	0
3	TRS	F	3249	8/8	0.21	4.06	60,60,60,61	0
3	TRS	B	3242	8/8	0.30	4.00	63,65,66,67	0
3	TRS	E	3253	8/8	0.32	3.24	62,62,62,62	0
3	TRS	A	3241	8/8	0.25	2.96	65,66,66,66	0
3	TRS	E	3247	8/8	0.23	2.52	47,47,48,49	0
3	TRS	F	3248	8/8	0.22	2.06	56,58,59,59	0
2	PLR	A	1500	15/15	0.11	0.23	26,27,27,28	0
2	PLR	B	1501	15/15	0.09	-0.35	23,24,26,26	0
2	PLR	C	1502	15/15	0.10	-0.36	18,22,22,23	0
2	PLR	E	1504	15/15	0.09	-0.37	17,21,22,22	0
2	PLR	F	1505	15/15	0.10	-0.46	20,24,25,27	0
2	PLR	D	1503	15/15	0.09	-0.50	23,27,29,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.