



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:59 AM UTC

PDB ID : 1SZK / pdb_00001szk
Title : The structure of gamma-aminobutyrate aminotransferase mutant: E211S
Authors : Liu, W.; Peterson, P.E.; Langston, J.A.; Jin, X.; Fisher, A.J.; Toney, M.D.
Deposited on : 2004-04-05
Resolution : 2.52 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

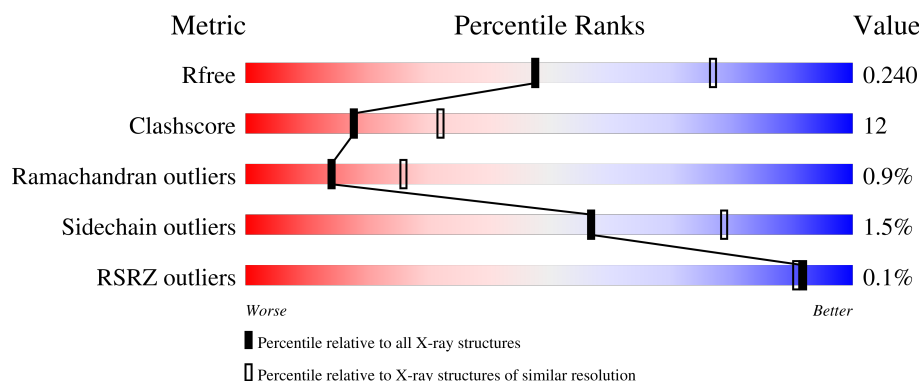
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	426	76% 22% .
1	B	426	75% 23% .
1	C	426	70% 29% .
1	D	426	67% 31% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	D	805	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13688 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 4-aminobutyrate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	1	0
			3209	2027	562	602	18			
1	B	425	Total	C	N	O	S	0	0	0
			3203	2024	561	600	18			
1	C	425	Total	C	N	O	S	0	0	0
			3203	2024	561	600	18			
1	D	425	Total	C	N	O	S	0	1	0
			3209	2027	562	602	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	SER	GLU	engineered mutation	UNP P22256
B	211	SER	GLU	engineered mutation	UNP P22256
C	211	SER	GLU	engineered mutation	UNP P22256
D	211	SER	GLU	engineered mutation	UNP P22256

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



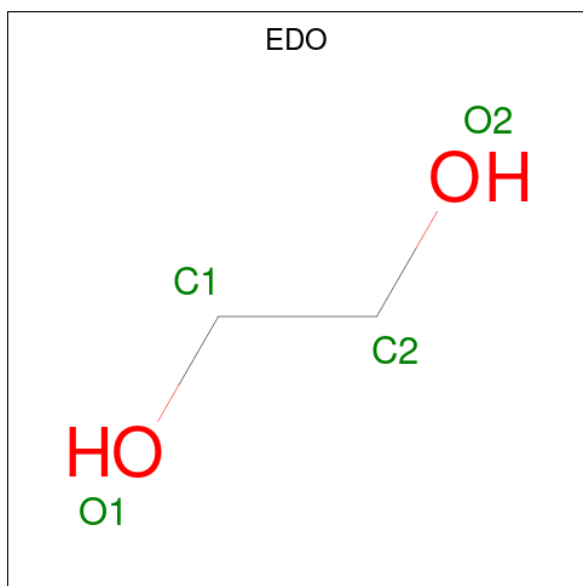
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



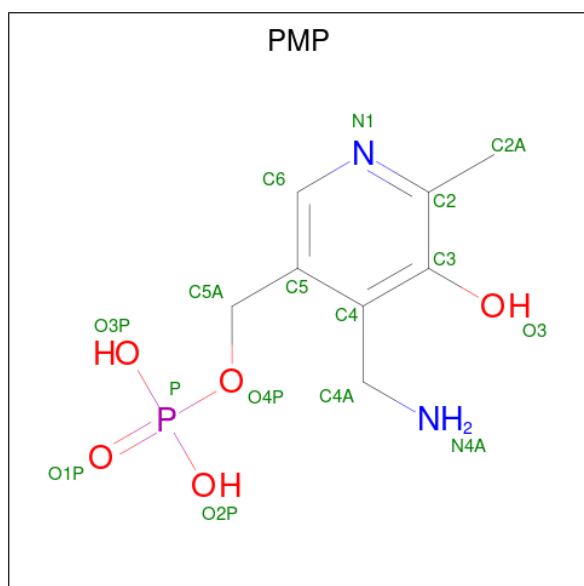
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: C₈H₁₃N₂O₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
4	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
4	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
4	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	179	Total	O	0	0
			179	179		
5	B	177	Total	O	0	0
			177	177		

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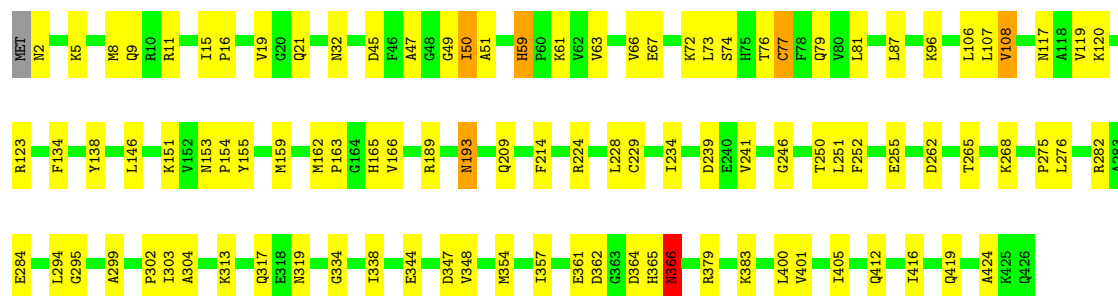
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	142	Total 142	O 142	0	0
5	D	175	Total 175	O 175	0	0

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.

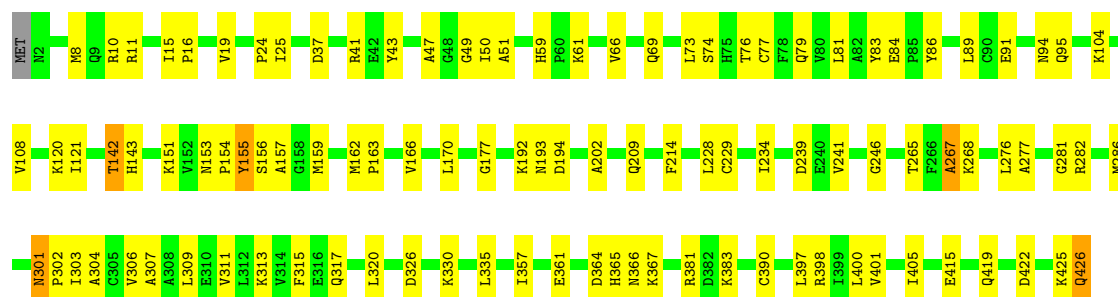
• Molecule 1: 4-aminobutyrate aminotransferase

Chain A: 



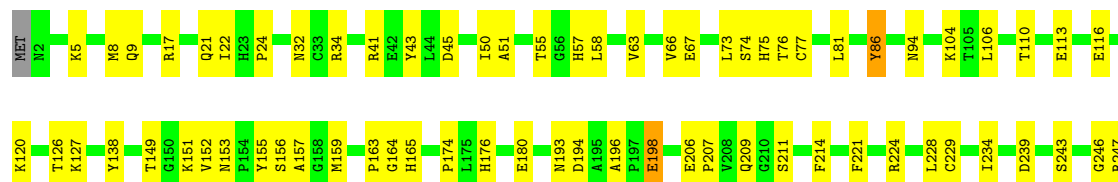
• Molecule 1: 4-aminobutyrate aminotransferase

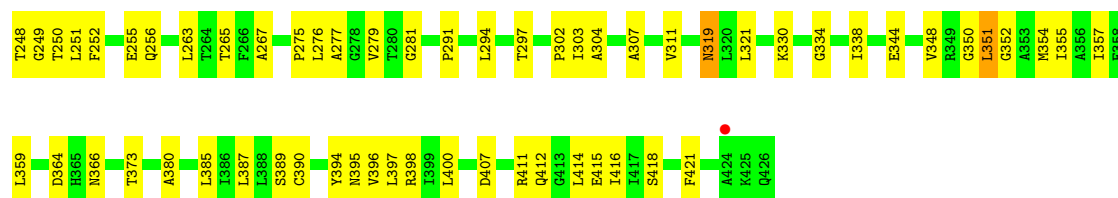
Chain B: 



• Molecule 1: 4-aminobutyrate aminotransferase

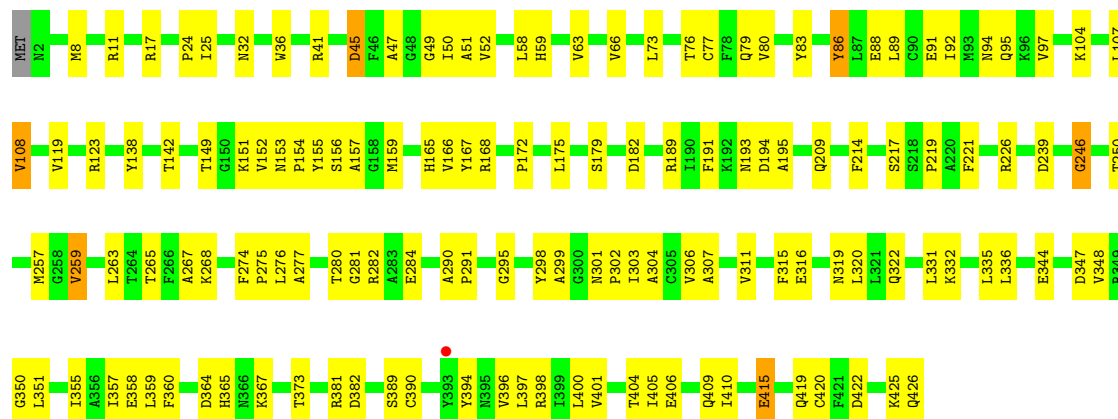
Chain C: 





• Molecule 1: 4-aminobutyrate aminotransferase

Chain D: 67% 31% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.26Å 108.26Å 300.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.52 30.00 – 2.52	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.52) 97.6 (30.00-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.187 , 0.240 0.187 , 0.240	Depositor DCC
R_{free} test set	3519 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13688	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PMP, EDO, SO4

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	0.45	0/3268	0.91	8/4423 (0.2%)
1	B	0.45	0/3262	0.93	10/4415 (0.2%)
1	C	0.44	0/3262	0.92	6/4415 (0.1%)
1	D	0.47	0/3268	0.94	10/4423 (0.2%)
All	All	0.45	0/13060	0.92	34/17676 (0.2%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	ASN	N-CA-C	7.90	121.41	111.69
1	C	194	ASP	N-CA-C	7.07	122.58	113.18
1	D	193	ASN	N-CA-C	6.80	121.91	112.45
1	D	166	VAL	N-CA-C	-6.73	98.69	108.11
1	A	166	VAL	N-CA-C	-6.59	98.02	107.77
1	B	194	ASP	N-CA-C	6.55	122.16	114.04
1	D	194	ASP	N-CA-C	6.49	122.09	114.04
1	C	411	ARG	N-CA-C	-6.32	104.32	111.14
1	B	301	ASN	CA-C-N	6.29	125.78	119.24
1	B	301	ASN	C-N-CA	6.29	125.78	119.24
1	C	297	THR	N-CA-C	6.18	118.52	111.11
1	D	45	ASP	N-CA-C	5.96	117.73	109.15
1	A	193	ASN	N-CA-C	5.89	120.64	112.45
1	D	301	ASN	CA-C-N	5.76	127.04	119.84
1	D	301	ASN	C-N-CA	5.76	127.04	119.84
1	B	84	GLU	N-CA-C	5.72	121.29	113.16
1	B	193	ASN	N-CA-C	5.62	120.14	113.12
1	A	45	ASP	N-CA-C	5.54	117.33	108.41
1	D	142	THR	N-CA-C	-5.47	102.42	110.52
1	D	295	GLY	N-CA-C	5.34	117.79	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	168	ARG	N-CA-C	5.33	118.30	109.46
1	B	202	ALA	N-CA-C	5.31	116.91	108.79
1	B	177	GLY	N-CA-C	5.29	121.37	115.08
1	D	246	GLY	N-CA-C	5.22	122.31	115.47
1	A	59	HIS	CA-C-N	5.21	124.65	119.24
1	A	59	HIS	C-N-CA	5.21	124.65	119.24
1	A	262	ASP	N-CA-C	-5.15	106.16	112.90
1	C	45	ASP	N-CA-C	5.12	116.61	108.67
1	C	75	HIS	N-CA-C	5.11	116.18	108.46
1	B	246	GLY	N-CA-C	5.07	122.11	115.47
1	B	142	THR	N-CA-C	-5.07	103.24	110.59
1	B	166	VAL	N-CA-C	-5.03	100.28	107.78
1	A	146	LEU	N-CA-C	-5.02	105.89	111.36
1	A	134	PHE	N-CA-C	5.01	117.91	110.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3209	0	3224	79	0
1	B	3203	0	3220	75	0
1	C	3203	0	3220	93	0
1	D	3209	0	3224	89	0
2	A	15	0	0	1	0
2	B	20	0	0	0	0
2	C	15	0	0	1	0
2	D	25	0	0	0	0
3	A	12	0	18	3	0
3	B	12	0	18	4	0
3	C	12	0	18	1	0
3	D	16	0	24	5	0
4	A	16	0	10	1	0
4	B	16	0	10	1	0
4	C	16	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	16	0	10	1	0
5	A	179	0	0	8	0
5	B	177	0	0	6	0
5	C	142	0	0	6	0
5	D	175	0	0	3	0
All	All	13688	0	13006	321	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 12.

All (321) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:ILE:HD11	1:D:381:ARG:HD3	1.43	1.00
1:B:25:ILE:HD11	1:B:381:ARG:HD3	1.45	0.98
1:C:243:SER:HA	1:C:354:MET:HE1	1.57	0.87
1:C:348:VAL:HG22	1:C:357:ILE:HG22	1.61	0.82
1:C:334:GLY:HA3	1:C:414:LEU:HD13	1.63	0.80
1:D:401:VAL:HG21	1:D:405:ILE:HD12	1.65	0.78
1:B:156:SER:HA	1:B:159:MET:HE3	1.67	0.76
1:C:17:ARG:HH11	1:D:291:PRO:HD3	1.51	0.75
1:A:401:VAL:HG21	1:A:405:ILE:HD12	1.68	0.74
1:A:165:HIS:H	3:C:803:EDO:H11	1.53	0.74
1:A:284:GLU:CD	1:A:284:GLU:H	1.99	0.70
1:C:350:GLY:HA3	1:C:355:ILE:HD13	1.74	0.70
1:D:364:ASP:OD2	1:D:367:LYS:HG3	1.91	0.70
5:A:857:HOH:O	1:C:157:ALA:HA	1.93	0.68
1:A:151:LYS:HD3	1:A:155:TYR:CE1	2.29	0.68
1:A:66:VAL:HG13	1:A:303:ILE:HG23	1.74	0.68
1:B:307:ALA:O	1:B:311:VAL:HG23	1.93	0.67
1:B:156:SER:HA	1:B:159:MET:CE	2.24	0.67
1:A:72:LYS:HE2	5:B:936:HOH:O	1.95	0.67
1:A:364:ASP:CG	1:A:366:ASN:HD21	2.03	0.66
1:B:151:LYS:HD3	1:B:155:TYR:CE1	2.31	0.65
1:B:151:LYS:HE3	1:B:153:ASN:O	1.95	0.65
1:D:88:GLU:O	1:D:92:ILE:HG13	1.97	0.65
1:D:41:ARG:HH22	1:D:382:ASP:C	2.05	0.64
1:C:196:ALA:HB1	1:C:198:GLU:OE2	1.98	0.63
1:A:366:ASN:N	1:A:366:ASN:HD22	1.96	0.63
1:C:17:ARG:NH1	1:D:291:PRO:HD3	2.13	0.63
1:C:76:THR:HB	3:D:805:EDO:H22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:GLY:HA2	1:C:250:THR:O	1.99	0.63
1:C:151:LYS:HE3	1:C:153:ASN:O	1.99	0.62
1:D:406:GLU:HB2	1:D:409:GLN:OE1	2.00	0.62
1:C:32:ASN:C	1:C:32:ASN:HD22	2.07	0.61
1:B:192:LYS:HD2	5:B:951:HOH:O	2.00	0.61
1:C:8:MET:HE1	1:C:21:GLN:HG2	1.82	0.61
1:A:63:VAL:O	1:A:67:GLU:HG3	2.01	0.60
1:C:256:GLN:OE1	1:C:351:LEU:HD21	2.01	0.60
1:B:8:MET:HE2	1:B:24:PRO:HB3	1.82	0.60
1:D:157:ALA:HA	5:D:940:HOH:O	2.00	0.60
1:B:426:GLN:N	1:B:426:GLN:NE2	2.50	0.59
1:C:265:THR:HG22	1:C:279:VAL:HG22	1.83	0.59
1:A:276:LEU:HB2	1:A:304:ALA:HB1	1.84	0.59
1:D:358:GLU:HG2	1:D:360:PHE:CE2	2.38	0.59
1:C:224:ARG:HD2	5:C:879:HOH:O	2.03	0.59
1:B:315:PHE:CD2	1:B:320:LEU:HB2	2.38	0.59
1:B:303:ILE:O	1:B:306:VAL:HG22	2.03	0.59
1:C:66:VAL:HG13	1:C:303:ILE:HG23	1.86	0.58
1:A:72:LYS:HD2	3:A:810:EDO:H12	1.85	0.58
1:B:157:ALA:HA	5:B:839:HOH:O	2.02	0.58
1:C:63:VAL:O	1:C:67:GLU:HG3	2.04	0.58
1:C:106:LEU:HD22	1:C:294:LEU:HD13	1.86	0.58
1:C:41:ARG:HG2	1:C:43:TYR:CE1	2.38	0.58
1:D:76:THR:O	1:D:77:CYS:HB3	2.04	0.58
1:D:47:ALA:HB3	3:D:805:EDO:O1	2.03	0.57
1:A:76:THR:HB	3:B:801:EDO:H11	1.86	0.57
1:A:313:LYS:HB3	1:A:317:GLN:HE21	1.69	0.57
1:B:229:CYS:HB3	1:B:234:ILE:O	2.06	0.56
1:C:412:GLN:O	1:C:416:ILE:HG13	2.06	0.56
1:C:229:CYS:HB3	1:C:234:ILE:O	2.06	0.56
1:B:361:GLU:HB2	1:B:367:LYS:CB	2.36	0.56
1:A:209:GLN:O	1:A:214:PHE:HA	2.06	0.55
1:B:426:GLN:N	1:B:426:GLN:HE21	2.04	0.55
1:D:350:GLY:HA3	1:D:355:ILE:HD13	1.87	0.55
1:B:361:GLU:HB2	1:B:367:LYS:HB3	1.88	0.55
1:D:209:GLN:O	1:D:214:PHE:HA	2.06	0.55
1:A:5:LYS:O	1:A:9:GLN:HG3	2.07	0.55
1:A:246:GLY:HA2	1:A:250:THR:O	2.07	0.55
1:A:162:MET:HB3	1:A:163:PRO:HD2	1.88	0.54
1:B:15:ILE:HG23	1:B:16:PRO:HD2	1.89	0.54
1:A:159:MET:HE2	1:B:120:LYS:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HD22	1:A:294:LEU:HD13	1.90	0.54
1:D:360:PHE:HB3	1:D:364:ASP:O	2.07	0.54
1:B:241:VAL:HG13	1:B:267:ALA:HB3	1.90	0.54
1:C:263:LEU:HD23	1:C:281:GLY:HA3	1.90	0.54
1:A:295:GLY:HA2	5:A:921:HOH:O	2.08	0.54
1:A:239:ASP:HA	1:A:265:THR:OG1	2.09	0.53
1:C:247:ARG:HG2	1:C:354:MET:HE3	1.90	0.53
1:A:282:ARG:NH2	5:A:968:HOH:O	2.41	0.53
1:B:209:GLN:O	1:B:214:PHE:HA	2.09	0.53
1:A:50:ILE:HG21	2:A:712:SO4:O2	2.09	0.53
5:C:923:HOH:O	1:D:58:LEU:HD13	2.07	0.53
1:D:94:ASN:HD21	1:D:104:LYS:C	2.17	0.53
1:B:37:ASP:OD2	1:B:41:ARG:HB3	2.08	0.53
1:C:344:GLU:H	1:C:344:GLU:CD	2.17	0.53
1:A:15:ILE:C	1:B:104:LYS:HD3	2.34	0.52
1:C:211:SER:HB3	2:C:714:SO4:O3	2.08	0.52
1:A:76:THR:O	1:A:77:CYS:HB3	2.10	0.52
1:D:415:GLU:O	1:D:419:GLN:HG3	2.08	0.52
1:D:51:ALA:HB2	1:D:400:LEU:HD22	1.92	0.52
1:C:359:LEU:HD21	1:C:421:PHE:HZ	1.75	0.52
1:D:390:CYS:SG	1:D:398:ARG:HD3	2.49	0.52
1:D:359:LEU:HD12	1:D:373:THR:HA	1.91	0.52
1:D:422:ASP:O	1:D:425:LYS:HG2	2.10	0.52
1:B:8:MET:HE2	1:B:24:PRO:CB	2.39	0.51
1:C:8:MET:HE2	1:C:24:PRO:HB3	1.91	0.51
1:A:2:ASN:N	5:A:966:HOH:O	2.43	0.51
1:C:5:LYS:O	1:C:9:GLN:HG3	2.10	0.51
1:C:110:THR:OG1	1:C:113:GLU:HG3	2.11	0.51
1:B:94:ASN:HD21	1:B:104:LYS:C	2.19	0.51
1:B:76:THR:O	1:B:77:CYS:HB3	2.11	0.51
1:D:316:GLU:HA	1:D:316:GLU:OE1	2.10	0.50
1:B:69:GLN:HG3	1:B:303:ILE:HD13	1.93	0.50
1:D:239:ASP:HA	1:D:265:THR:OG1	2.10	0.50
1:D:389:SER:HA	1:D:396:VAL:O	2.11	0.50
1:A:383:LYS:HE3	1:A:419:GLN:HB3	1.92	0.50
1:B:66:VAL:HG13	1:B:303:ILE:HG23	1.94	0.50
1:A:138:TYR:HE2	4:A:750:PMP:HNA1	1.54	0.50
1:B:383:LYS:HE3	1:B:419:GLN:HB3	1.93	0.50
1:B:426:GLN:NE2	1:B:426:GLN:H	2.09	0.50
1:D:303:ILE:O	1:D:306:VAL:HG22	2.12	0.49
1:D:406:GLU:O	1:D:410:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:CYS:SG	1:C:398:ARG:HD3	2.51	0.49
1:D:360:PHE:CD1	1:D:365:HIS:HA	2.47	0.49
1:A:108:VAL:HG12	5:A:930:HOH:O	2.12	0.49
1:B:214:PHE:HZ	1:B:400:LEU:HD21	1.77	0.49
1:C:17:ARG:NH1	1:D:291:PRO:CD	2.75	0.49
1:C:55:THR:HG21	1:C:311:VAL:HG13	1.95	0.49
1:C:180:GLU:HG2	1:C:221:PHE:HB2	1.94	0.49
1:C:276:LEU:HG	1:C:277:ALA:N	2.26	0.49
1:B:364:ASP:C	1:B:366:ASN:H	2.20	0.49
1:C:380:ALA:HB1	1:C:385:LEU:HB3	1.93	0.49
1:C:138:TYR:HA	1:C:149:THR:HG23	1.94	0.49
1:A:252:PHE:O	1:A:255:GLU:HG3	2.12	0.49
1:C:276:LEU:HB2	1:C:304:ALA:HB1	1.94	0.49
1:C:66:VAL:HG13	1:C:303:ILE:CG2	2.43	0.49
1:A:77:CYS:SG	1:A:79:GLN:HG2	2.53	0.49
1:B:74:SER:O	1:B:302:PRO:HD2	2.12	0.49
1:C:17:ARG:NH1	1:D:290:ALA:HA	2.27	0.49
1:D:394:TYR:CD1	1:D:394:TYR:N	2.80	0.49
1:A:96:LYS:HB3	1:A:251:LEU:HD23	1.94	0.49
1:B:228:LEU:C	1:B:228:LEU:HD23	2.38	0.49
1:D:268:LYS:NZ	4:D:753:PMP:N4A	2.60	0.49
1:C:34:ARG:NH1	5:C:909:HOH:O	2.46	0.48
1:A:366:ASN:HD22	1:A:366:ASN:H	1.59	0.48
1:B:79:GLN:HG3	5:B:862:HOH:O	2.12	0.48
1:D:32:ASN:C	1:D:32:ASN:HD22	2.21	0.48
1:C:116:GLU:O	1:C:120:LYS:HG3	2.13	0.48
1:B:268:LYS:CE	4:B:751:PMP:H4A2	2.43	0.48
1:D:97:VAL:HB	1:D:280:THR:HG21	1.96	0.48
1:A:412:GLN:O	1:A:416:ILE:HG13	2.12	0.48
1:C:94:ASN:HD21	1:C:104:LYS:C	2.21	0.48
1:A:81:LEU:HD22	3:B:801:EDO:H12	1.96	0.47
1:D:11:ARG:HH11	1:D:11:ARG:HG2	1.79	0.47
1:A:282:ARG:HG2	1:A:284:GLU:OE1	2.14	0.47
1:B:89:LEU:HA	1:B:309:LEU:HD21	1.95	0.47
1:D:79:GLN:HG3	5:D:855:HOH:O	2.15	0.47
1:D:281:GLY:O	1:D:282:ARG:C	2.57	0.47
1:D:52:VAL:HG22	1:D:268:LYS:HA	1.96	0.47
1:D:167:TYR:HA	3:D:812:EDO:H11	1.97	0.47
1:C:164:GLY:O	1:C:165:HIS:HB2	2.14	0.47
1:D:36:TRP:HA	1:D:41:ARG:O	2.14	0.47
1:A:120:LYS:NZ	5:A:846:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ASN:N	1:A:366:ASN:ND2	2.57	0.47
1:C:76:THR:O	1:C:77:CYS:HB3	2.13	0.47
1:C:214:PHE:CZ	1:C:398:ARG:HB2	2.50	0.47
1:C:248:THR:HB	1:C:351:LEU:HD22	1.97	0.47
1:D:32:ASN:ND2	1:D:404:THR:OG1	2.47	0.47
1:B:239:ASP:HA	1:B:265:THR:OG1	2.15	0.47
1:A:334:GLY:O	1:A:338:ILE:HG13	2.14	0.47
1:C:86:TYR:C	1:C:86:TYR:CD2	2.92	0.47
1:C:126:THR:O	1:C:127:LYS:HB2	2.13	0.47
1:C:364:ASP:C	1:C:366:ASN:H	2.23	0.47
1:C:51:ALA:HB2	1:C:400:LEU:HD22	1.97	0.47
1:C:152:VAL:HG13	1:C:156:SER:HB2	1.96	0.47
1:B:364:ASP:OD1	1:B:367:LYS:HE3	2.15	0.47
1:D:108:VAL:HG23	1:D:277:ALA:HB3	1.96	0.47
1:D:83:TYR:CE1	1:D:86:TYR:HB2	2.51	0.46
1:B:426:GLN:HG2	1:B:426:GLN:O	2.15	0.46
1:D:151:LYS:HE2	1:D:153:ASN:O	2.15	0.46
1:A:15:ILE:HG23	1:A:16:PRO:HD2	1.96	0.46
1:D:66:VAL:HG13	1:D:303:ILE:HG23	1.97	0.46
1:D:219:PRO:HD2	5:D:862:HOH:O	2.14	0.46
1:B:83:TYR:CE1	1:B:86:TYR:HB2	2.49	0.46
1:C:73:LEU:HD12	1:C:73:LEU:C	2.40	0.46
1:D:175:LEU:O	1:D:175:LEU:HG	2.14	0.46
1:D:155:TYR:O	1:D:159:MET:HE1	2.15	0.46
1:D:263:LEU:HD23	1:D:281:GLY:HA3	1.96	0.46
1:B:281:GLY:O	1:B:282:ARG:C	2.58	0.46
1:B:422:ASP:O	1:B:425:LYS:HB2	2.16	0.46
1:D:138:TYR:HA	1:D:149:THR:HG23	1.97	0.46
1:A:11:ARG:HH22	1:A:19:VAL:HG12	1.81	0.46
1:A:59:HIS:O	1:A:63:VAL:HG23	2.16	0.46
1:A:282:ARG:NH1	5:A:913:HOH:O	2.33	0.46
1:B:47:ALA:HB3	3:B:801:EDO:O2	2.16	0.46
1:C:228:LEU:C	1:C:228:LEU:HD23	2.41	0.45
1:A:49:GLY:HA2	1:B:76:THR:O	2.15	0.45
1:A:119:VAL:O	1:A:123:ARG:HG3	2.15	0.45
1:D:347:ASP:O	1:D:357:ILE:HA	2.16	0.45
1:A:364:ASP:OD2	1:A:366:ASN:ND2	2.41	0.45
1:B:73:LEU:C	1:B:73:LEU:HD12	2.42	0.45
1:B:108:VAL:HG23	1:B:277:ALA:HB3	1.98	0.45
1:D:59:HIS:O	1:D:63:VAL:HG23	2.16	0.45
1:D:73:LEU:C	1:D:73:LEU:HD12	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:MET:HB3	1:A:163:PRO:CD	2.46	0.45
1:D:91:GLU:O	1:D:95:GLN:HG2	2.16	0.45
1:A:151:LYS:HE3	1:A:153:ASN:O	2.17	0.45
1:B:170:LEU:HD21	1:D:189:ARG:HD3	1.99	0.45
1:C:120:LYS:NZ	5:C:846:HOH:O	2.39	0.45
1:A:241:VAL:HG12	1:A:268:LYS:HE2	1.99	0.45
1:B:66:VAL:HG13	1:B:303:ILE:CG2	2.47	0.45
1:C:86:TYR:C	1:C:86:TYR:HD2	2.25	0.45
1:D:344:GLU:CD	1:D:344:GLU:H	2.25	0.45
1:B:91:GLU:O	1:B:95:GLN:HG2	2.17	0.45
1:C:319:ASN:ND2	5:C:855:HOH:O	2.50	0.45
1:B:11:ARG:HG2	1:B:11:ARG:HH11	1.82	0.45
1:A:107:LEU:O	1:A:299:ALA:HB1	2.17	0.44
1:C:81:LEU:HD22	3:D:805:EDO:H21	1.99	0.44
1:A:32:ASN:HD22	1:A:32:ASN:C	2.24	0.44
1:C:32:ASN:C	1:C:32:ASN:ND2	2.73	0.44
1:D:73:LEU:HD12	1:D:73:LEU:O	2.17	0.44
1:A:74:SER:HA	1:A:303:ILE:CD1	2.47	0.44
1:A:108:VAL:HG11	1:A:117:ASN:ND2	2.33	0.44
1:D:172:PRO:HG3	1:D:221:PHE:CD2	2.53	0.44
1:D:284:GLU:OE2	1:D:284:GLU:N	2.39	0.44
1:B:51:ALA:HB2	1:B:400:LEU:HD22	2.00	0.44
1:B:276:LEU:HB2	1:B:304:ALA:HB1	1.99	0.44
1:A:73:LEU:HD12	1:A:73:LEU:C	2.42	0.44
1:B:282:ARG:HD3	5:B:950:HOH:O	2.18	0.44
1:C:373:THR:OG1	1:C:395:ASN:HA	2.18	0.44
1:A:106:LEU:HD13	1:B:19:VAL:CG2	2.48	0.44
1:A:344:GLU:H	1:A:344:GLU:CD	2.26	0.44
1:B:301:ASN:HA	1:B:302:PRO:HD3	1.87	0.44
1:B:121:ILE:HD13	1:B:286:MET:CE	2.48	0.43
3:B:804:EDO:H11	1:D:165:HIS:H	1.83	0.43
1:C:174:PRO:C	1:C:176:HIS:H	2.26	0.43
1:A:229:CYS:HB3	1:A:234:ILE:O	2.19	0.43
1:C:249:GLY:O	1:C:321:LEU:HD22	2.18	0.43
1:A:379:ARG:NE	1:A:424:ALA:HB2	2.34	0.43
1:B:170:LEU:HD21	1:D:189:ARG:CD	2.48	0.43
1:C:357:ILE:O	1:C:357:ILE:HG13	2.17	0.43
1:C:94:ASN:HD22	1:C:94:ASN:HA	1.66	0.43
1:C:239:ASP:HA	1:C:265:THR:OG1	2.19	0.43
1:C:385:LEU:CD2	1:C:387:LEU:HD21	2.48	0.43
1:B:326:ASP:O	1:B:330:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:GLU:O	1:C:207:PRO:C	2.62	0.43
1:C:338:ILE:HD13	1:C:418:SER:HA	2.00	0.43
1:D:179:SER:O	1:D:182:ASP:N	2.51	0.43
1:A:189:ARG:O	1:A:193:ASN:HB2	2.19	0.43
1:A:47:ALA:HB3	3:A:808:EDO:O2	2.19	0.43
1:C:55:THR:HG23	5:C:870:HOH:O	2.18	0.43
1:C:34:ARG:HG3	1:C:34:ARG:HH11	1.83	0.42
1:C:41:ARG:HG2	1:C:43:TYR:CZ	2.53	0.42
1:C:214:PHE:CE1	1:C:398:ARG:HD2	2.54	0.42
1:C:334:GLY:HA3	1:C:414:LEU:CD1	2.43	0.42
1:C:8:MET:HE2	1:C:24:PRO:CB	2.49	0.42
1:A:361:GLU:O	1:A:362:ASP:HB2	2.20	0.42
1:B:61:LYS:HE3	1:B:317:GLN:OE1	2.20	0.42
1:B:390:CYS:SG	1:B:398:ARG:HD3	2.59	0.42
1:C:359:LEU:HD12	1:C:373:THR:HA	2.02	0.42
1:D:49:GLY:HA2	3:D:805:EDO:H12	2.00	0.42
1:D:298:TYR:O	1:D:299:ALA:C	2.63	0.42
1:A:228:LEU:C	1:A:228:LEU:HD23	2.45	0.42
1:C:319:ASN:HD22	1:C:319:ASN:HA	1.68	0.42
1:A:74:SER:O	1:A:302:PRO:HD2	2.20	0.42
1:A:347:ASP:O	1:A:357:ILE:HA	2.19	0.42
1:A:224:ARG:HD2	5:A:914:HOH:O	2.20	0.42
1:A:303:ILE:HD12	1:A:303:ILE:H	1.85	0.42
3:A:808:EDO:C1	1:B:81:LEU:HD12	2.50	0.42
1:D:86:TYR:CD2	1:D:107:LEU:HD12	2.55	0.42
1:D:332:LYS:HG3	1:D:348:VAL:HG12	2.00	0.42
1:C:22:ILE:HB	1:D:80:VAL:HA	2.02	0.42
1:C:174:PRO:C	1:C:176:HIS:N	2.76	0.42
1:A:76:THR:O	1:B:49:GLY:HA2	2.19	0.42
1:B:357:ILE:HD11	1:B:397:LEU:HD12	2.02	0.42
1:D:322:GLN:HA	1:D:322:GLN:NE2	2.34	0.42
1:C:291:PRO:HA	1:D:17:ARG:O	2.20	0.42
1:D:226:ARG:HG2	1:D:259:VAL:HG22	2.01	0.42
1:D:422:ASP:O	1:D:426:GLN:HG3	2.20	0.42
1:C:248:THR:C	1:C:352:GLY:HA3	2.45	0.41
1:B:59:HIS:CE1	1:B:61:LYS:HB2	2.56	0.41
1:C:155:TYR:O	1:C:159:MET:HE1	2.19	0.41
1:D:191:PHE:HA	1:D:195:ALA:O	2.20	0.41
1:A:303:ILE:HD12	1:A:303:ILE:N	2.35	0.41
1:B:357:ILE:O	1:B:357:ILE:HG13	2.21	0.41
1:D:152:VAL:HG13	1:D:156:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:HD12	1:A:251:LEU:HA	1.91	0.41
1:C:17:ARG:HH12	1:D:290:ALA:HA	1.84	0.41
1:D:331:LEU:O	1:D:335:LEU:HG	2.21	0.41
1:D:357:ILE:HD11	1:D:397:LEU:HD12	2.02	0.41
1:A:364:ASP:O	1:A:366:ASN:N	2.42	0.41
1:B:401:VAL:HG21	1:B:405:ILE:HD12	2.02	0.41
1:A:87:LEU:HD21	1:B:10:ARG:HB2	2.01	0.41
1:A:348:VAL:HG22	1:A:357:ILE:HG22	2.03	0.41
1:C:74:SER:O	1:C:302:PRO:HD2	2.20	0.41
1:D:307:ALA:O	1:D:311:VAL:HG23	2.20	0.41
1:B:335:LEU:HD13	1:B:357:ILE:CG2	2.51	0.41
1:C:57:HIS:O	1:C:58:LEU:C	2.64	0.41
1:C:348:VAL:HG22	1:C:357:ILE:CG2	2.42	0.41
1:C:389:SER:HA	1:C:396:VAL:O	2.20	0.41
1:D:76:THR:O	1:D:77:CYS:CB	2.69	0.41
1:A:51:ALA:HB2	1:A:400:LEU:HD22	2.03	0.41
1:A:153:ASN:HA	1:A:154:PRO:HA	1.89	0.41
1:B:162:MET:HB3	1:B:163:PRO:CD	2.51	0.41
1:B:162:MET:HB3	1:B:163:PRO:HD2	2.03	0.41
1:B:313:LYS:O	1:B:317:GLN:HG2	2.21	0.41
1:C:307:ALA:O	1:C:311:VAL:HG23	2.20	0.41
1:D:217:SER:O	1:D:257:MET:HE1	2.21	0.41
1:D:332:LYS:O	1:D:336:LEU:HG	2.21	0.41
1:A:32:ASN:C	1:A:32:ASN:ND2	2.79	0.41
1:B:11:ARG:NH1	5:B:920:HOH:O	2.54	0.41
1:C:344:GLU:CD	1:C:344:GLU:N	2.79	0.41
1:D:246:GLY:HA2	1:D:250:THR:O	2.20	0.41
1:D:276:LEU:HB2	1:D:304:ALA:HB1	2.03	0.41
1:B:43:TYR:CD1	1:B:43:TYR:N	2.89	0.40
1:B:142:THR:O	1:B:143:HIS:C	2.65	0.40
1:C:252:PHE:O	1:C:255:GLU:HG3	2.21	0.40
1:C:330:LYS:NZ	1:C:407:ASP:OD1	2.53	0.40
1:C:209:GLN:O	1:C:214:PHE:HA	2.21	0.40
1:D:8:MET:HE2	1:D:24:PRO:HB3	2.04	0.40
1:D:45:ASP:OD1	1:D:45:ASP:C	2.65	0.40
1:D:274:PHE:HA	1:D:275:PRO:HD3	1.91	0.40
1:D:351:LEU:HD23	1:D:351:LEU:HA	1.97	0.40
1:A:59:HIS:HE1	1:A:61:LYS:HG2	1.86	0.40
1:A:250:THR:O	1:A:251:LEU:C	2.65	0.40
1:A:379:ARG:HE	1:A:424:ALA:HB2	1.86	0.40
1:B:364:ASP:OD1	1:B:367:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:PHE:CD2	1:D:320:LEU:HB2	2.56	0.40
1:C:357:ILE:HD11	1:C:397:LEU:HD12	2.02	0.40
1:A:8:MET:HE1	1:A:21:GLN:HG2	2.03	0.40
1:C:251:LEU:HD12	1:C:251:LEU:HA	1.94	0.40
1:D:119:VAL:O	1:D:123:ARG:HG3	2.21	0.40
1:D:419:GLN:O	1:D:420:CYS:C	2.65	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	424/426 (100%)	395 (93%)	23 (5%)	6 (1%)	9	16
1	B	423/426 (99%)	393 (93%)	26 (6%)	4 (1%)	14	26
1	C	423/426 (99%)	394 (93%)	26 (6%)	3 (1%)	18	32
1	D	424/426 (100%)	391 (92%)	30 (7%)	3 (1%)	18	32
All	All	1694/1704 (99%)	1573 (93%)	105 (6%)	16 (1%)	14	26

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	HIS
1	B	155	TYR
1	B	365	HIS
1	D	50	ILE
1	B	267	ALA
1	A	50	ILE
1	A	77	CYS
1	A	366	ASN
1	B	50	ILE

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Mol	Chain	Res	Type
1	C	275	PRO
1	D	267	ALA
1	C	267	ALA
1	D	108	VAL
1	A	275	PRO
1	C	50	ILE
1	A	108	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	330/330 (100%)	327 (99%)	3 (1%)	70	86
1	B	329/330 (100%)	326 (99%)	3 (1%)	70	86
1	C	329/330 (100%)	322 (98%)	7 (2%)	47	72
1	D	330/330 (100%)	323 (98%)	7 (2%)	47	72
All	All	1318/1320 (100%)	1298 (98%)	20 (2%)	57	79

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	ASN
1	A	354	MET
1	A	366	ASN
1	B	154	PRO
1	B	415	GLU
1	B	426	GLN
1	C	86	TYR
1	C	163	PRO
1	C	198	GLU
1	C	319	ASN
1	C	351	LEU
1	C	394	TYR
1	C	415	GLU
1	D	86	TYR

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Mol	Chain	Res	Type
1	D	89	LEU
1	D	154	PRO
1	D	259	VAL
1	D	302	PRO
1	D	319	ASN
1	D	415	GLU

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

Mol	Chain	Res	Type
1	A	9	GLN
1	A	32	ASN
1	A	94	ASN
1	A	117	ASN
1	A	188	HIS
1	A	317	GLN
1	A	319	ASN
1	A	329	GLN
1	A	366	ASN
1	A	419	GLN
1	B	13	GLN
1	B	32	ASN
1	B	94	ASN
1	B	117	ASN
1	B	242	GLN
1	B	366	ASN
1	B	426	GLN
1	C	2	ASN
1	C	32	ASN
1	C	94	ASN
1	C	95	GLN
1	C	232	HIS
1	C	242	GLN
1	C	317	GLN
1	C	319	ASN
1	C	329	GLN
1	C	365	HIS
1	D	32	ASN
1	D	94	ASN
1	D	176	HIS
1	D	242	GLN
1	D	319	ASN

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Mol	Chain	Res	Type
1	D	322	GLN
1	D	365	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

32 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	SO4	D	711	-	4,4,4	1.86	2 (50%)	6,6,6	0.83	0
3	EDO	A	810	-	3,3,3	0.49	0	2,2,2	0.39	0
2	SO4	B	713	-	4,4,4	1.85	2 (50%)	6,6,6	0.84	0
3	EDO	A	813	-	3,3,3	0.49	0	2,2,2	0.41	0
2	SO4	B	702	-	4,4,4	1.90	2 (50%)	6,6,6	0.81	0
2	SO4	D	705	-	4,4,4	1.87	2 (50%)	6,6,6	0.84	0
2	SO4	C	710	-	4,4,4	1.86	2 (50%)	6,6,6	0.84	0
2	SO4	D	709	-	4,4,4	1.87	2 (50%)	6,6,6	0.80	0
3	EDO	B	802	-	3,3,3	0.56	0	2,2,2	0.36	0
4	PMP	A	750	-	16,16,16	4.72	4 (25%)	22,23,23	1.58	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	811	-	3,3,3	0.53	0	2,2,2	0.41	0
3	EDO	D	807	-	3,3,3	0.47	0	2,2,2	0.42	0
4	PMP	D	753	-	16,16,16	4.73	6 (37%)	22,23,23	1.56	3 (13%)
2	SO4	A	707	-	4,4,4	1.86	2 (50%)	6,6,6	0.82	0
2	SO4	B	708	-	4,4,4	1.86	2 (50%)	6,6,6	0.82	0
2	SO4	C	704	-	4,4,4	1.88	2 (50%)	6,6,6	0.83	0
2	SO4	A	712	-	4,4,4	1.82	2 (50%)	6,6,6	0.83	0
3	EDO	B	801	-	3,3,3	0.52	0	2,2,2	0.33	0
2	SO4	D	715	-	4,4,4	1.87	2 (50%)	6,6,6	0.82	0
2	SO4	C	714	-	4,4,4	1.85	2 (50%)	6,6,6	0.83	0
2	SO4	B	703	-	4,4,4	1.85	2 (50%)	6,6,6	0.85	0
3	EDO	D	805	-	3,3,3	0.45	0	2,2,2	0.40	0
3	EDO	B	804	-	3,3,3	0.54	0	2,2,2	0.38	0
3	EDO	C	803	-	3,3,3	0.52	0	2,2,2	0.37	0
2	SO4	D	706	-	4,4,4	1.84	2 (50%)	6,6,6	0.85	0
3	EDO	C	809	-	3,3,3	0.50	0	2,2,2	0.34	0
3	EDO	D	812	-	3,3,3	0.44	0	2,2,2	0.45	0
3	EDO	D	806	-	3,3,3	0.53	0	2,2,2	0.40	0
4	PMP	C	752	-	16,16,16	4.83	4 (25%)	22,23,23	1.57	2 (9%)
2	SO4	A	701	-	4,4,4	1.87	2 (50%)	6,6,6	0.82	0
4	PMP	B	751	-	16,16,16	4.81	5 (31%)	22,23,23	1.65	3 (13%)
3	EDO	A	808	-	3,3,3	0.48	0	2,2,2	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	806	-	-	1/1/1/1	-
3	EDO	D	807	-	-	0/1/1/1	-
4	PMP	C	752	-	-	2/8/8/8	0/1/1/1
4	PMP	D	753	-	-	1/8/8/8	0/1/1/1
3	EDO	D	805	-	-	0/1/1/1	-
3	EDO	B	804	-	-	1/1/1/1	-
4	PMP	A	750	-	-	0/8/8/8	0/1/1/1
3	EDO	A	810	-	-	1/1/1/1	-
3	EDO	A	813	-	-	0/1/1/1	-
4	PMP	B	751	-	-	0/8/8/8	0/1/1/1
3	EDO	C	803	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	809	-	-	1/1/1/1	-
3	EDO	B	802	-	-	0/1/1/1	-
3	EDO	A	808	-	-	0/1/1/1	-
3	EDO	B	801	-	-	0/1/1/1	-
3	EDO	D	812	-	-	1/1/1/1	-
3	EDO	C	811	-	-	1/1/1/1	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	753	PMP	C5-C4	13.98	1.60	1.40
4	A	750	PMP	C5-C4	13.81	1.59	1.40
4	C	752	PMP	C5-C4	13.80	1.59	1.40
4	B	751	PMP	C5-C4	13.70	1.59	1.40
4	C	752	PMP	C3-C2	11.40	1.52	1.41
4	B	751	PMP	C3-C2	10.88	1.52	1.41
4	A	750	PMP	C3-C2	10.74	1.52	1.41
4	D	753	PMP	C3-C2	9.99	1.51	1.41
4	B	751	PMP	C6-N1	5.28	1.45	1.34
4	D	753	PMP	C6-N1	5.04	1.44	1.34
4	C	752	PMP	C6-N1	4.78	1.44	1.34
4	A	750	PMP	C6-N1	4.51	1.43	1.34
4	D	753	PMP	C2-N1	4.42	1.41	1.33
4	B	751	PMP	C2-N1	4.36	1.41	1.33
4	A	750	PMP	C2-N1	4.16	1.41	1.33
4	C	752	PMP	C2-N1	4.11	1.41	1.33
2	B	702	SO4	O1-S	3.13	1.63	1.44
2	D	705	SO4	O1-S	3.10	1.63	1.44
2	A	701	SO4	O1-S	3.10	1.63	1.44
2	C	704	SO4	O1-S	3.10	1.63	1.44
2	B	703	SO4	O1-S	3.07	1.63	1.44
2	D	709	SO4	O1-S	3.07	1.63	1.44
2	D	711	SO4	O1-S	3.07	1.63	1.44
2	C	710	SO4	O1-S	3.06	1.63	1.44
2	B	708	SO4	O1-S	3.05	1.63	1.44
2	A	707	SO4	O1-S	3.05	1.63	1.44
2	D	715	SO4	O1-S	3.03	1.62	1.44
2	C	714	SO4	O1-S	3.03	1.62	1.44
2	D	706	SO4	O1-S	3.02	1.62	1.44
2	B	713	SO4	O1-S	2.98	1.62	1.44
2	A	712	SO4	O1-S	2.92	1.62	1.44
4	B	751	PMP	C2A-C2	2.61	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	715	SO4	O3-S	-2.14	1.30	1.48
2	B	713	SO4	O3-S	-2.14	1.30	1.48
2	A	712	SO4	O3-S	-2.13	1.30	1.48
2	D	709	SO4	O3-S	-2.10	1.30	1.48
2	C	714	SO4	O3-S	-2.09	1.30	1.48
2	B	702	SO4	O3-S	-2.09	1.31	1.48
2	B	708	SO4	O3-S	-2.08	1.31	1.48
2	C	704	SO4	O3-S	-2.08	1.31	1.48
2	A	707	SO4	O3-S	-2.08	1.31	1.48
2	C	710	SO4	O3-S	-2.07	1.31	1.48
2	D	711	SO4	O3-S	-2.07	1.31	1.48
2	D	706	SO4	O3-S	-2.07	1.31	1.48
2	A	701	SO4	O3-S	-2.05	1.31	1.48
2	D	705	SO4	O3-S	-2.05	1.31	1.48
2	B	703	SO4	O3-S	-2.03	1.31	1.48
4	D	753	PMP	P-O3P	-2.00	1.47	1.54
4	D	753	PMP	C2A-C2	2.00	1.53	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	751	PMP	C2A-C2-C3	5.04	126.69	120.80
4	A	750	PMP	C2A-C2-C3	5.03	126.69	120.80
4	C	752	PMP	C2A-C2-C3	4.79	126.41	120.80
4	D	753	PMP	C2A-C2-C3	4.51	126.08	120.80
4	B	751	PMP	C3-C2-N1	-2.51	117.80	120.96
4	D	753	PMP	C6-N1-C2	2.19	123.16	119.20
4	D	753	PMP	C3-C2-N1	-2.17	118.22	120.96
4	A	750	PMP	C3-C2-N1	-2.16	118.23	120.96
4	C	752	PMP	C3-C2-N1	-2.06	118.36	120.96
4	B	751	PMP	C6-N1-C2	2.05	122.91	119.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	752	PMP	C3-C4-C4A-N4A
4	C	752	PMP	C5-C4-C4A-N4A
4	D	753	PMP	C3-C4-C4A-N4A
3	A	810	EDO	O1-C1-C2-O2
3	C	811	EDO	O1-C1-C2-O2
3	C	803	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	D	812	EDO	O1-C1-C2-O2
3	B	804	EDO	O1-C1-C2-O2
3	C	809	EDO	O1-C1-C2-O2
3	D	806	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	810	EDO	1	0
4	A	750	PMP	1	0
4	D	753	PMP	1	0
2	A	712	SO4	1	0
3	B	801	EDO	3	0
2	C	714	SO4	1	0
3	D	805	EDO	4	0
3	B	804	EDO	1	0
3	C	803	EDO	1	0
3	D	812	EDO	1	0
4	B	751	PMP	1	0
3	A	808	EDO	2	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 [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	425/426 (99%)	-0.42	0	100 100	10, 32, 57, 86	1 (0%)
1	B	425/426 (99%)	-0.38	0	100 100	17, 32, 69, 97	0
1	C	425/426 (99%)	-0.20	1 (0%)	91 90	17, 39, 79, 100	0
1	D	425/426 (99%)	-0.38	1 (0%)	91 90	9, 31, 66, 94	1 (0%)
All	All	1700/1704 (99%)	-0.35	2 (0%)	92 91	9, 33, 70, 100	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	424	ALA	2.7
1	D	393	TYR	2.3

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	SO4	D	711	5/5	0.53	0.14	130,130,130,131	0
2	SO4	B	702	5/5	0.73	0.15	94,94,95,95	0
2	SO4	B	708	5/5	0.75	0.12	106,107,107,107	0
2	SO4	D	709	5/5	0.76	0.16	101,101,102,102	0
2	SO4	C	710	5/5	0.76	0.16	94,94,95,95	0
2	SO4	B	703	5/5	0.77	0.14	96,97,97,98	0
2	SO4	A	701	5/5	0.81	0.14	114,114,114,115	0
2	SO4	C	704	5/5	0.82	0.11	100,100,101,101	0
2	SO4	B	713	5/5	0.83	0.18	117,117,118,118	0
2	SO4	D	706	5/5	0.83	0.12	110,110,110,110	0
2	SO4	A	707	5/5	0.84	0.10	113,113,114,114	0
2	SO4	A	712	5/5	0.85	0.18	120,120,120,120	0
2	SO4	D	715	5/5	0.85	0.18	119,120,120,120	0
2	SO4	D	705	5/5	0.86	0.13	88,88,88,88	0
3	EDO	A	810	4/4	0.88	0.13	53,56,57,57	0
3	EDO	B	804	4/4	0.90	0.12	50,50,51,54	0
2	SO4	C	714	5/5	0.91	0.12	106,107,107,107	0
3	EDO	C	803	4/4	0.91	0.13	50,50,51,55	0
3	EDO	D	807	4/4	0.91	0.12	53,54,54,56	0
3	EDO	B	802	4/4	0.92	0.08	38,41,43,43	0
3	EDO	A	813	4/4	0.92	0.11	49,50,51,52	0
3	EDO	D	812	4/4	0.92	0.10	33,34,37,37	0
3	EDO	D	805	4/4	0.93	0.16	42,42,43,45	0
3	EDO	B	801	4/4	0.94	0.10	47,47,48,48	0
3	EDO	C	809	4/4	0.94	0.14	53,55,56,57	0
3	EDO	C	811	4/4	0.94	0.11	31,32,33,34	0
3	EDO	A	808	4/4	0.95	0.11	51,52,52,53	0
4	PMP	C	752	16/16	0.96	0.07	25,31,36,37	0
4	PMP	A	750	16/16	0.97	0.07	24,28,32,35	0
4	PMP	B	751	16/16	0.97	0.06	18,28,32,34	0
3	EDO	D	806	4/4	0.97	0.09	52,55,55,57	0
4	PMP	D	753	16/16	0.98	0.05	21,24,32,34	0

6.5 Other polymers

There are no such residues in this entry.