



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2017 – 07:43 PM EDT

PDB ID : 1LQF
Title : Structure of PTP1b in Complex with a Peptidic Bisphosphonate Inhibitor
Authors : Asante-Appiah, E.; Patel, S.; Dufresne, C.; Scapin, G.
Deposited on : unknown
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

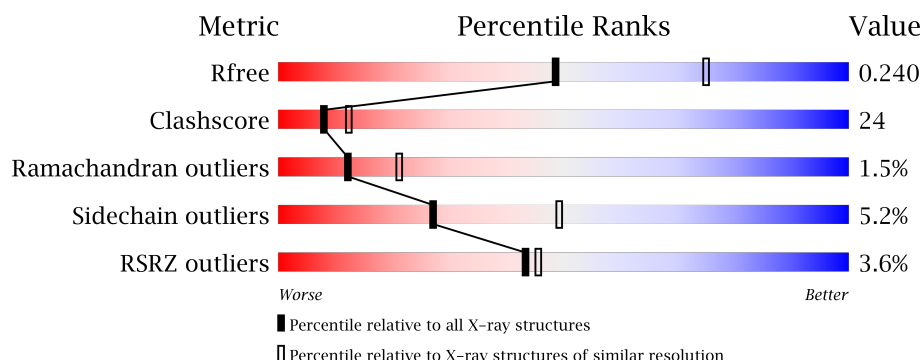
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	295	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>34%</div> <div>• •</div> </div> </div>
1	B	295	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>• •</div> </div> </div>
1	C	295	<div> <div>6%</div> <div> <div></div> <div>59%</div> <div>33%</div> <div>5% •</div> </div> </div>
1	D	295	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>34%</div> <div>• •</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGD	A	802	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10076 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 protein-tyrosine phosphatase, non-receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2336	1483	402	435	16			
1	B	287	Total	C	N	O	S	0	0	0
			2335	1483	401	435	16			
1	C	287	Total	C	N	O	S	0	0	0
			2322	1472	401	433	16			
1	D	287	Total	C	N	O	S	0	0	0
			2339	1486	402	435	16			

There are 48 discrepancies between the modelled and reference sequences:

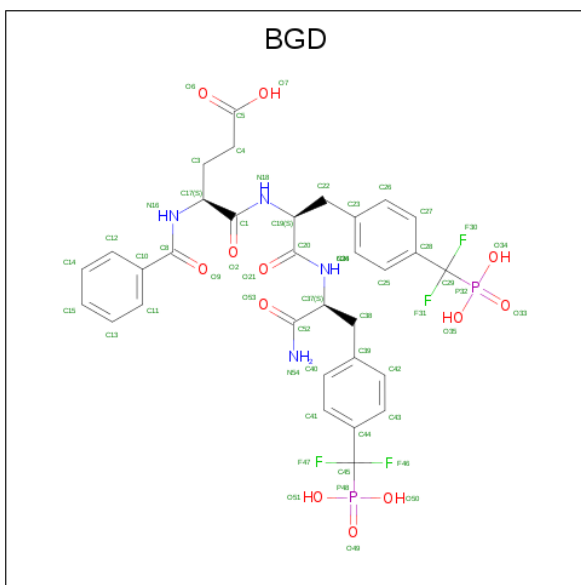
Chain	Residue	Modelled	Actual	Comment	Reference
A	489	MET	-	see remark 999	UNP P18031
A	490	ASP	-	see remark 999	UNP P18031
A	491	TYR	-	see remark 999	UNP P18031
A	492	LYS	-	see remark 999	UNP P18031
A	493	ASP	-	see remark 999	UNP P18031
A	494	ASP	-	see remark 999	UNP P18031
A	495	ASP	-	see remark 999	UNP P18031
A	496	ASP	-	see remark 999	UNP P18031
A	497	LYS	-	see remark 999	UNP P18031
A	498	LEU	-	see remark 999	UNP P18031
A	499	GLU	-	see remark 999	UNP P18031
A	500	PHE	-	see remark 999	UNP P18031
B	489	MET	-	see remark 999	UNP P18031
B	490	ASP	-	see remark 999	UNP P18031
B	491	TYR	-	see remark 999	UNP P18031
B	492	LYS	-	see remark 999	UNP P18031
B	493	ASP	-	see remark 999	UNP P18031
B	494	ASP	-	see remark 999	UNP P18031
B	495	ASP	-	see remark 999	UNP P18031
B	496	ASP	-	see remark 999	UNP P18031
B	497	LYS	-	see remark 999	UNP P18031

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Chain	Residue	Modelled	Actual	Comment	Reference
B	498	LEU	-	see remark 999	UNP P18031
B	499	GLU	-	see remark 999	UNP P18031
B	500	PHE	-	see remark 999	UNP P18031
C	489	MET	-	see remark 999	UNP P18031
C	490	ASP	-	see remark 999	UNP P18031
C	491	TYR	-	see remark 999	UNP P18031
C	492	LYS	-	see remark 999	UNP P18031
C	493	ASP	-	see remark 999	UNP P18031
C	494	ASP	-	see remark 999	UNP P18031
C	495	ASP	-	see remark 999	UNP P18031
C	496	ASP	-	see remark 999	UNP P18031
C	497	LYS	-	see remark 999	UNP P18031
C	498	LEU	-	see remark 999	UNP P18031
C	499	GLU	-	see remark 999	UNP P18031
C	500	PHE	-	see remark 999	UNP P18031
D	489	MET	-	see remark 999	UNP P18031
D	490	ASP	-	see remark 999	UNP P18031
D	491	TYR	-	see remark 999	UNP P18031
D	492	LYS	-	see remark 999	UNP P18031
D	493	ASP	-	see remark 999	UNP P18031
D	494	ASP	-	see remark 999	UNP P18031
D	495	ASP	-	see remark 999	UNP P18031
D	496	ASP	-	see remark 999	UNP P18031
D	497	LYS	-	see remark 999	UNP P18031
D	498	LEU	-	see remark 999	UNP P18031
D	499	GLU	-	see remark 999	UNP P18031
D	500	PHE	-	see remark 999	UNP P18031

- Molecule 2 is N-BENZOYL-L-GLUTAMYL-[4-PHOSPHONO(DIFLUOROMETHYL)]-L-PHENYLALANINE-[4-PHOSPHONO(DIFLUORO-METHYL)]-L-PHENYLALANINEAMIDE (three-letter code: BGD) (formula: C₃₂H₃₄F₄N₄O₁₂P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 54	C 32	F 4	N 4	O 12	P 2	0	0
2	B	1	Total 54	C 32	F 4	N 4	O 12	P 2	0	0
2	C	1	Total 54	C 32	F 4	N 4	O 12	P 2	0	0
2	D	1	Total 54	C 32	F 4	N 4	O 12	P 2	0	0

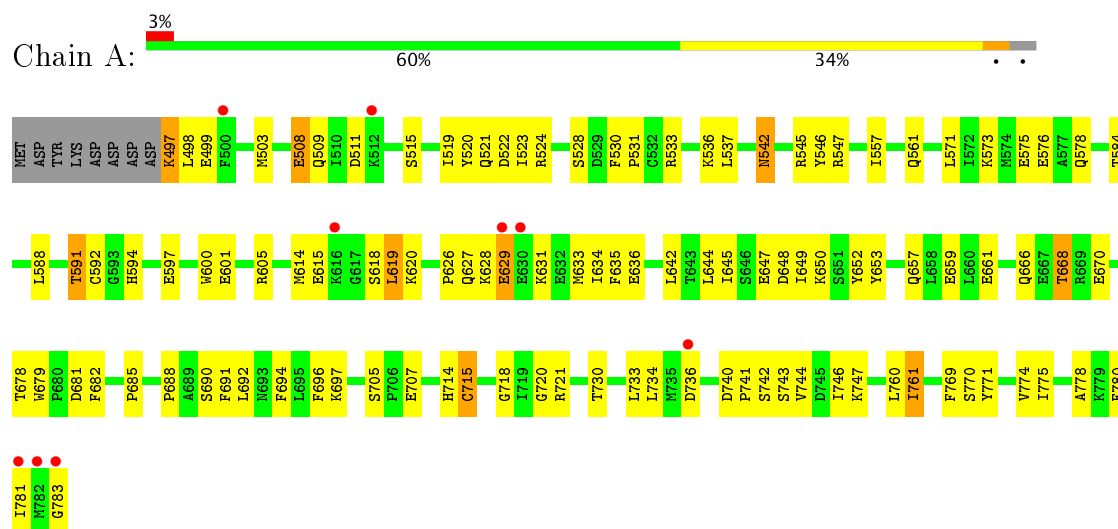
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	129	Total O 129 129	0	0
3	B	176	Total O 176 176	0	0
3	C	126	Total O 126 126	0	0
3	D	97	Total O 97 97	0	0

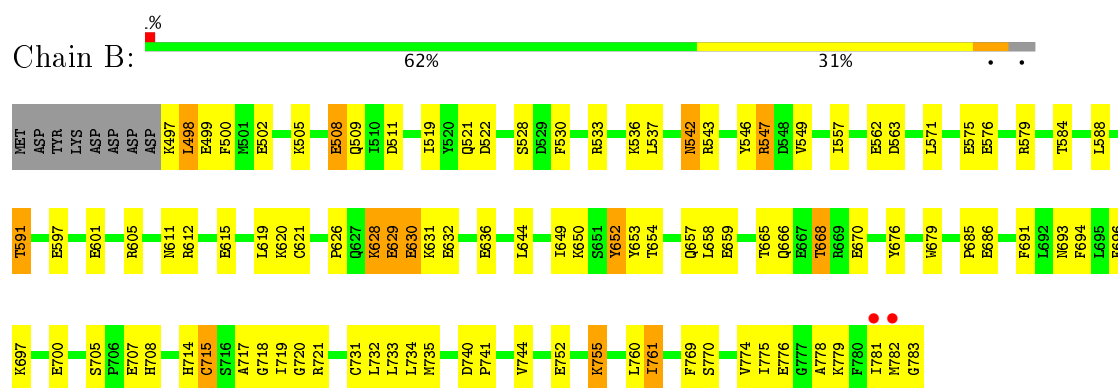
3 Residue-property plots

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

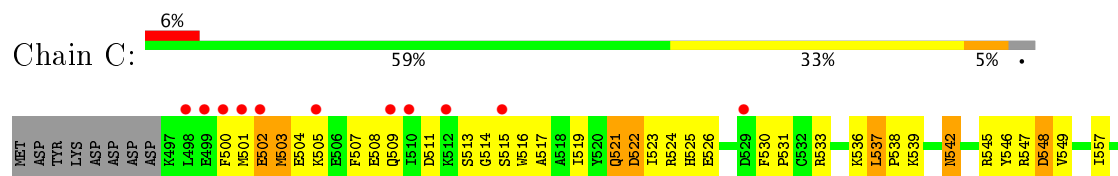
- Molecule 1: protein-tyrosine phosphatase, non-receptor type 1

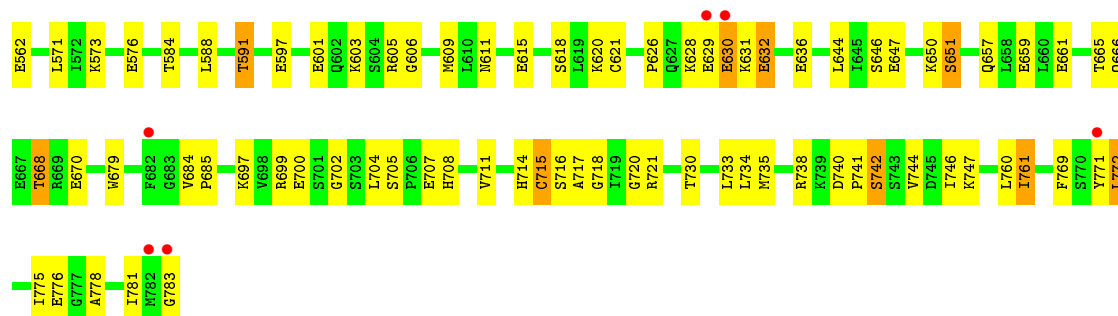


- Molecule 1: protein-tyrosine phosphatase, non-receptor type 1

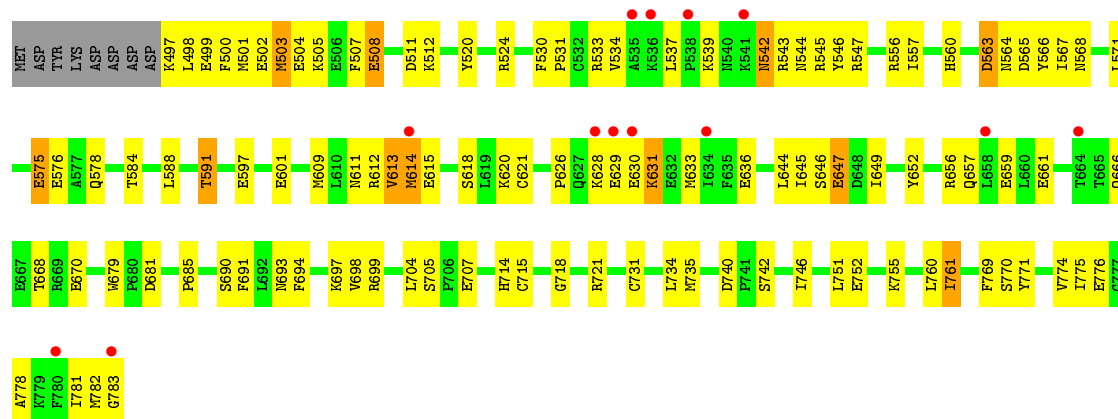


- Molecule 1: protein-tyrosine phosphatase, non-receptor type 1





- Molecule 1: protein-tyrosine phosphatase, non-receptor type 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.87Å 154.42Å 64.60Å 90.00° 94.56° 90.00°	Depositor
Resolution (Å)	29.00 – 2.50 39.71 – 2.41	Depositor EDS
% Data completeness (in resolution range)	91.4 (29.00-2.50) 90.9 (39.71-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.286 0.242 , 0.240	Depositor DCC
R_{free} test set	3093 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10076	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: BGD

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	0.58	0/2389	0.71	0/3218
1	B	0.66	0/2388	0.75	0/3218
1	C	0.61	0/2374	0.73	1/3200 (0.0%)
1	D	0.56	0/2392	0.70	0/3222
All	All	0.60	0/9543	0.72	1/12858 (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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	772	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	652	TYR	Sidechain

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	2336	0	2297	112	0
1	B	2335	0	2295	96	0
1	C	2322	0	2275	124	0
1	D	2339	0	2306	125	0
2	A	54	0	27	6	0
2	B	54	0	29	2	0
2	C	54	0	27	5	0
2	D	54	0	29	3	0
3	A	129	0	0	17	0
3	B	176	0	0	10	0
3	C	126	0	0	19	0
3	D	97	0	0	11	0
All	All	10076	0	9285	448	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 24.

All (448) 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:B:498:LEU:HD12	1:B:498:LEU:H	1.29	0.98
1:B:563:ASP:HB3	3:B:3302:HOH:O	1.63	0.97
1:B:547:ARG:NH1	1:B:547:ARG:HB3	1.79	0.97
1:C:628:LYS:HB2	1:C:628:LYS:NZ	1.80	0.96
1:B:591:THR:HG21	3:B:3140:HOH:O	1.64	0.95
1:A:499:GLU:HG2	1:A:740:ASP:OD1	1.67	0.94
1:C:502:GLU:O	1:C:505:LYS:HB3	1.67	0.94
1:D:613:VAL:HG12	1:D:621:CYS:O	1.69	0.93
1:D:597:GLU:O	1:D:601:GLU:HG3	1.67	0.93
1:D:498:LEU:O	1:D:498:LEU:HD13	1.67	0.92
1:A:670:GLU:HG3	3:A:3013:HOH:O	1.69	0.92
1:D:539:LYS:HE2	1:D:564:ASN:HD22	1.35	0.90
1:A:770:SER:O	1:A:774:VAL:HG23	1.70	0.90
1:D:556:ARG:HB2	3:D:3237:HOH:O	1.71	0.89
1:B:693:ASN:HB2	3:B:3129:HOH:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3044:HOH:O	1:C:562:GLU:HB3	1.74	0.87
1:C:538:PRO:HD2	3:C:3175:HOH:O	1.73	0.86
1:C:597:GLU:O	1:C:601:GLU:HG3	1.75	0.86
1:B:770:SER:O	1:B:774:VAL:HG23	1.75	0.85
1:C:628:LYS:HB2	1:C:628:LYS:HZ2	1.40	0.85
1:D:693:ASN:O	1:D:697:LYS:HG2	1.78	0.84
1:A:597:GLU:O	1:A:601:GLU:HG3	1.79	0.83
1:D:626:PRO:HG3	1:D:633:MET:HG3	1.60	0.83
1:C:615:GLU:HB2	1:C:620:LYS:HG3	1.63	0.81
1:C:500:PHE:HA	3:C:3403:HOH:O	1.79	0.81
1:A:627:GLN:H	1:A:631:LYS:HD3	1.47	0.80
1:B:707:GLU:OE2	1:C:708:HIS:CE1	2.34	0.80
1:B:659:GLU:OE2	1:B:668:THR:HB	1.81	0.79
1:A:521:GLN:HA	1:A:524:ARG:HD3	1.65	0.79
1:A:533:ARG:HG3	1:A:533:ARG:HH11	1.47	0.79
1:B:533:ARG:HH11	1:B:533:ARG:HG3	1.48	0.79
1:A:780:PHE:O	1:D:693:ASN:ND2	2.16	0.79
1:D:631:LYS:HE2	1:D:631:LYS:HA	1.64	0.79
1:C:533:ARG:HG3	1:C:533:ARG:HH11	1.49	0.78
1:A:659:GLU:OE2	1:A:668:THR:HB	1.80	0.78
1:C:659:GLU:OE2	1:C:668:THR:HB	1.83	0.77
1:D:588:LEU:HB2	1:D:591:THR:HB	1.66	0.76
1:A:626:PRO:HB2	1:A:644:LEU:HB2	1.65	0.76
1:C:666:GLN:HG3	3:C:3292:HOH:O	1.84	0.76
1:B:708:HIS:NE2	1:C:707:GLU:OE1	2.19	0.75
1:C:697:LYS:HE2	3:C:3472:HOH:O	1.86	0.75
1:B:497:LYS:C	1:B:499:GLU:H	1.86	0.75
1:B:597:GLU:O	1:B:601:GLU:HG3	1.86	0.75
1:D:659:GLU:OE2	1:D:668:THR:HB	1.87	0.75
1:C:705:SER:OG	1:C:707:GLU:HG2	1.88	0.74
1:D:615:GLU:HB2	1:D:620:LYS:HG3	1.69	0.73
1:B:547:ARG:HH11	1:B:547:ARG:HB3	1.52	0.73
1:D:614:MET:HA	1:D:618:SER:O	1.87	0.73
1:A:705:SER:OG	1:A:707:GLU:HG2	1.88	0.73
1:D:533:ARG:HG3	1:D:533:ARG:HH11	1.54	0.72
1:A:746:ILE:HG13	1:A:771:TYR:CE2	2.25	0.72
1:C:628:LYS:HE3	1:C:631:LYS:HD3	1.71	0.72
1:A:678:THR:HG22	3:A:3017:HOH:O	1.89	0.72
1:B:499:GLU:OE1	1:B:741:PRO:HD2	1.90	0.72
1:D:705:SER:OG	1:D:707:GLU:HG2	1.90	0.71
1:C:628:LYS:CE	1:C:631:LYS:HD3	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:GLN:HG3	1:C:524:ARG:HH22	1.57	0.70
1:B:752:GLU:O	1:B:755:LYS:HB2	1.92	0.70
1:D:770:SER:O	1:D:774:VAL:HG23	1.92	0.69
1:D:539:LYS:CE	1:D:564:ASN:HD22	2.05	0.69
1:B:611:ASN:HB2	1:B:615:GLU:OE2	1.92	0.69
1:A:647:GLU:O	1:A:649:ILE:HD12	1.92	0.69
1:A:497:LYS:HE2	1:A:499:GLU:OE1	1.92	0.69
1:C:628:LYS:HA	3:C:3295:HOH:O	1.93	0.69
1:D:694:PHE:O	1:D:698:VAL:HG23	1.92	0.69
1:B:497:LYS:O	1:B:499:GLU:N	2.26	0.69
1:D:543:ARG:NH2	1:D:564:ASN:HB3	2.07	0.69
1:D:539:LYS:HE2	1:D:564:ASN:ND2	2.05	0.68
1:B:652:TYR:CE1	1:B:686:GLU:HG3	2.28	0.68
1:C:629:GLU:O	1:C:630:GLU:HB2	1.93	0.68
1:D:497:LYS:HE3	3:D:3244:HOH:O	1.94	0.68
1:D:631:LYS:HA	1:D:631:LYS:CE	2.23	0.68
1:C:685:PRO:HD2	1:C:769:PHE:CE2	2.29	0.67
1:A:594:HIS:CD2	3:A:3511:HOH:O	2.47	0.67
1:C:628:LYS:NZ	1:C:631:LYS:HD3	2.10	0.66
1:A:653:TYR:OH	1:A:697:LYS:NZ	2.29	0.66
1:D:752:GLU:HA	1:D:755:LYS:HE2	1.77	0.65
1:B:696:PHE:HE2	1:B:700:GLU:OE1	1.80	0.65
1:B:502:GLU:O	1:B:505:LYS:HB3	1.96	0.65
1:C:605:ARG:HG3	1:C:708:HIS:CE1	2.32	0.65
1:D:629:GLU:HG2	1:D:630:GLU:H	1.60	0.65
1:D:584:THR:O	1:D:714:HIS:HB2	1.97	0.65
1:C:523:ILE:HD11	1:C:747:LYS:HD2	1.77	0.65
1:B:528:SER:OG	1:B:755:LYS:HD2	1.97	0.65
1:C:525:HIS:O	3:C:3160:HOH:O	2.15	0.64
1:C:626:PRO:HB2	1:C:644:LEU:HB2	1.79	0.64
1:A:515:SER:HB3	3:A:3361:HOH:O	1.96	0.64
1:A:666:GLN:HG2	3:A:3434:HOH:O	1.96	0.64
1:D:647:GLU:OE1	1:D:649:ILE:HD11	1.97	0.64
1:C:679:TRP:CE2	1:C:721:ARG:HG2	2.32	0.63
1:D:499:GLU:HB3	1:D:742:SER:OG	1.98	0.63
1:B:696:PHE:CE2	1:B:700:GLU:OE1	2.51	0.63
1:A:645:ILE:HD11	1:A:659:GLU:HB2	1.80	0.63
1:C:533:ARG:HD3	3:D:3483:HOH:O	1.97	0.63
1:A:688:PRO:HG3	1:A:769:PHE:HE1	1.63	0.62
1:D:534:VAL:HG21	3:D:3456:HOH:O	1.98	0.62
1:A:627:GLN:N	1:A:631:LYS:HD3	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:500:PHE:HA	1:D:503:MET:HG2	1.80	0.62
1:A:545:ARG:HG2	1:A:546:TYR:CE1	2.35	0.62
1:A:679:TRP:CE2	1:A:721:ARG:HG2	2.34	0.62
1:D:626:PRO:HB2	1:D:644:LEU:HB2	1.82	0.62
1:A:588:LEU:HB2	1:A:591:THR:HB	1.80	0.62
1:A:575:GLU:OE2	1:A:575:GLU:N	2.26	0.62
1:C:501:MET:HA	1:C:504:GLU:OE2	1.99	0.62
1:A:742:SER:HB2	3:A:3443:HOH:O	2.00	0.62
1:C:523:ILE:CD1	1:C:747:LYS:HD2	2.29	0.62
1:D:545:ARG:HH21	1:D:620:LYS:C	2.02	0.62
1:C:521:GLN:HG3	1:C:524:ARG:NH2	2.15	0.61
1:D:545:ARG:HD3	1:D:546:TYR:CE1	2.34	0.61
1:A:573:LYS:HE2	3:A:3069:HOH:O	2.00	0.61
1:C:537:LEU:HD12	3:C:3226:HOH:O	2.00	0.61
1:B:497:LYS:O	1:B:782:MET:CE	2.48	0.61
1:D:679:TRP:CE2	1:D:721:ARG:HG2	2.36	0.61
1:A:615:GLU:HB2	1:A:620:LYS:CG	2.30	0.61
1:C:545:ARG:HH11	1:C:545:ARG:HG3	1.65	0.61
1:B:509:GLN:HE21	1:B:509:GLN:HA	1.66	0.60
1:A:509:GLN:HA	1:A:509:GLN:HE21	1.67	0.60
1:C:588:LEU:HB2	1:C:591:THR:HB	1.82	0.60
1:D:557:ILE:HD11	1:D:571:LEU:HB2	1.83	0.60
1:D:499:GLU:HG2	1:D:740:ASP:OD1	2.01	0.60
1:D:666:GLN:NE2	3:D:3415:HOH:O	2.33	0.60
1:B:629:GLU:C	1:B:631:LYS:H	2.05	0.60
1:A:615:GLU:HB2	1:A:620:LYS:HG3	1.83	0.59
1:D:626:PRO:HB3	1:D:631:LYS:HB3	1.83	0.59
1:B:547:ARG:HB3	1:B:547:ARG:CZ	2.32	0.59
1:B:629:GLU:O	1:B:631:LYS:N	2.35	0.59
1:C:509:GLN:HA	1:C:509:GLN:HE21	1.67	0.59
1:D:628:LYS:HG2	1:D:631:LYS:HD2	1.85	0.59
1:D:544:ASN:OD1	1:D:566:TYR:OH	2.17	0.59
1:D:507:PHE:HD2	1:D:771:TYR:CD2	2.20	0.59
1:B:498:LEU:CD1	1:B:498:LEU:H	2.06	0.59
1:C:502:GLU:HG3	1:C:503:MET:N	2.17	0.59
1:B:500:PHE:HZ	1:B:779:LYS:HZ1	1.51	0.59
1:B:752:GLU:HB2	3:B:3420:HOH:O	2.03	0.59
1:C:503:MET:O	1:C:507:PHE:N	2.27	0.58
1:C:629:GLU:OE1	1:C:646:SER:HA	2.03	0.58
1:A:685:PRO:HD2	1:A:769:PHE:CE2	2.36	0.58
1:B:497:LYS:O	1:B:782:MET:HE2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:499:GLU:O	1:D:502:GLU:HB3	2.03	0.58
1:C:538:PRO:HD3	3:C:3265:HOH:O	2.03	0.58
1:D:507:PHE:HD2	1:D:771:TYR:HD2	1.50	0.58
1:D:751:LEU:HD12	3:D:3234:HOH:O	2.03	0.58
1:B:707:GLU:OE2	1:C:708:HIS:NE2	2.36	0.58
1:B:499:GLU:HG2	1:B:502:GLU:OE2	2.04	0.57
1:C:670:GLU:HG3	3:C:3293:HOH:O	2.04	0.57
1:B:498:LEU:HD12	1:B:498:LEU:N	2.11	0.57
1:A:746:ILE:HB	1:A:771:TYR:CZ	2.40	0.57
1:B:497:LYS:C	1:B:499:GLU:N	2.57	0.57
1:B:562:GLU:N	3:B:3365:HOH:O	2.38	0.57
1:C:628:LYS:HB2	1:C:628:LYS:HZ3	1.68	0.57
1:A:628:LYS:O	1:A:629:GLU:HB2	2.04	0.57
1:B:679:TRP:CE2	1:B:721:ARG:HG2	2.39	0.57
1:B:533:ARG:HG3	1:B:533:ARG:NH1	2.19	0.57
1:A:618:SER:HB3	2:A:802:BGD:H15	1.87	0.56
1:A:690:SER:HB2	3:A:3009:HOH:O	2.05	0.56
1:C:657:GLN:NE2	1:C:670:GLU:OE2	2.39	0.56
1:A:561:GLN:NE2	3:A:3511:HOH:O	2.38	0.56
1:D:542:ASN:H	1:D:542:ASN:HD22	1.53	0.56
1:A:573:LYS:NZ	3:A:3424:HOH:O	2.37	0.56
1:B:547:ARG:CB	1:B:547:ARG:CZ	2.83	0.56
1:D:500:PHE:O	1:D:504:GLU:HG3	2.06	0.56
1:A:533:ARG:HG3	1:A:533:ARG:NH1	2.20	0.56
1:D:629:GLU:HG2	1:D:630:GLU:N	2.20	0.55
1:D:752:GLU:HB2	3:D:3249:HOH:O	2.06	0.55
1:A:600:TRP:HE1	1:C:562:GLU:CD	2.09	0.55
1:D:628:LYS:O	1:D:631:LYS:HB2	2.06	0.55
1:B:615:GLU:HB2	1:B:620:LYS:HG3	1.88	0.55
1:A:688:PRO:HG3	1:A:769:PHE:CE1	2.41	0.55
1:D:685:PRO:HD2	1:D:769:PHE:CZ	2.41	0.55
1:B:546:TYR:CD2	2:B:803:BGD:H382	2.41	0.55
1:A:736:ASP:OD2	1:D:697:LYS:NZ	2.40	0.55
1:C:603:LYS:HB3	1:C:605:ARG:HH12	1.70	0.55
1:D:661:GLU:HB2	1:D:668:THR:HG22	1.88	0.55
1:A:576:GLU:HG2	1:A:734:LEU:CD2	2.37	0.55
1:A:576:GLU:HG2	1:A:734:LEU:HD21	1.89	0.55
1:C:630:GLU:C	1:C:632:GLU:H	2.10	0.54
1:D:497:LYS:HB2	1:D:499:GLU:OE1	2.07	0.54
1:D:647:GLU:HG3	1:D:656:ARG:HG2	1.89	0.54
1:D:576:GLU:HG2	1:D:734:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:LYS:HD2	1:A:498:LEU:H	1.73	0.54
1:B:546:TYR:CZ	2:B:803:BGD:H42	2.43	0.54
1:A:720:GLY:HA3	3:A:3068:HOH:O	2.06	0.53
1:C:549:VAL:HG21	1:C:717:ALA:HB1	1.90	0.53
1:D:545:ARG:NE	1:D:620:LYS:O	2.40	0.53
1:B:628:LYS:O	1:B:631:LYS:HB3	2.09	0.53
1:A:633:MET:HE3	1:A:635:PHE:CZ	2.43	0.53
1:C:548:ASP:OD1	2:C:804:BGD:H381	2.08	0.53
1:C:603:LYS:O	1:C:605:ARG:NH1	2.41	0.53
1:D:576:GLU:HG2	1:D:734:LEU:CD2	2.38	0.53
1:C:545:ARG:NH1	1:C:545:ARG:HG3	2.23	0.53
1:D:498:LEU:C	1:D:500:PHE:H	2.10	0.53
1:B:591:THR:O	1:B:591:THR:CG2	2.56	0.53
1:D:500:PHE:C	1:D:502:GLU:N	2.62	0.53
1:A:497:LYS:HB3	1:A:499:GLU:OE1	2.09	0.53
1:D:542:ASN:N	1:D:542:ASN:HD22	2.04	0.53
1:B:705:SER:OG	1:B:707:GLU:HG2	2.08	0.53
1:D:645:ILE:HG22	1:D:646:SER:N	2.23	0.52
1:C:573:LYS:HD3	3:C:3027:HOH:O	2.09	0.52
1:A:547:ARG:HH11	1:A:547:ARG:HG2	1.73	0.52
1:A:521:GLN:NE2	1:A:524:ARG:HD3	2.24	0.52
1:C:519:ILE:HA	1:C:522:ASP:OD2	2.10	0.52
1:A:594:HIS:HD2	3:A:3511:HOH:O	1.85	0.52
1:A:619:LEU:HD22	3:A:3063:HOH:O	2.09	0.52
1:B:500:PHE:CE1	1:B:775:ILE:O	2.62	0.52
1:C:630:GLU:H	1:C:644:LEU:HB3	1.74	0.52
1:A:547:ARG:HG2	1:A:547:ARG:NH1	2.25	0.52
1:D:575:GLU:O	1:D:578:GLN:N	2.42	0.52
1:A:584:THR:O	1:A:714:HIS:HB2	2.10	0.51
1:B:498:LEU:C	1:B:500:PHE:H	2.11	0.51
1:A:547:ARG:HG3	2:A:802:BGD:O2	2.10	0.51
1:C:618:SER:OG	2:C:804:BGD:H15	2.11	0.51
1:D:560:HIS:HB2	1:D:601:GLU:OE2	2.10	0.51
1:B:731:CYS:O	1:B:735:MET:HG3	2.09	0.51
1:C:684:VAL:HG23	3:C:3191:HOH:O	2.10	0.51
1:C:746:ILE:HB	1:C:771:TYR:CZ	2.46	0.51
1:A:633:MET:O	1:A:634:ILE:HG13	2.11	0.51
1:A:619:LEU:O	2:A:802:BGD:H13	2.11	0.51
1:B:500:PHE:HE1	1:B:775:ILE:O	1.93	0.51
1:C:548:ASP:OD2	2:C:804:BGD:H19	2.11	0.51
1:D:545:ARG:HD3	1:D:546:TYR:HE1	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:611:ASN:HD21	1:C:621:CYS:HB2	1.75	0.50
1:C:628:LYS:CB	1:C:628:LYS:NZ	2.63	0.50
1:B:557:ILE:HD11	1:B:571:LEU:HB2	1.93	0.50
1:B:588:LEU:HB2	1:B:591:THR:HB	1.94	0.50
1:A:547:ARG:HD2	2:A:802:BGD:H41A	1.94	0.50
1:A:520:TYR:O	1:A:524:ARG:HG3	2.10	0.50
1:B:630:GLU:HA	1:B:630:GLU:OE2	2.12	0.50
1:C:715:CYS:SG	1:C:718:GLY:HA2	2.52	0.50
1:C:704:LEU:HB2	3:C:3173:HOH:O	2.11	0.50
1:D:542:ASN:H	1:D:542:ASN:ND2	2.09	0.50
1:C:502:GLU:HG3	1:C:503:MET:H	1.77	0.50
1:D:563:ASP:OD1	1:D:564:ASN:N	2.45	0.49
1:D:567:ILE:HA	3:D:3235:HOH:O	2.11	0.49
1:D:545:ARG:NH2	1:D:620:LYS:C	2.65	0.49
1:A:633:MET:HE2	1:A:642:LEU:HD23	1.93	0.49
1:D:565:ASP:CG	1:D:565:ASP:O	2.50	0.49
1:A:592:CYS:N	3:A:3070:HOH:O	2.45	0.49
1:D:498:LEU:C	1:D:500:PHE:N	2.63	0.49
1:B:509:GLN:NE2	1:B:509:GLN:HA	2.28	0.49
1:B:649:ILE:HG12	1:B:654:THR:OG1	2.12	0.49
1:C:738:ARG:NH1	1:C:744:VAL:HA	2.25	0.49
1:D:505:LYS:O	1:D:508:GLU:HB3	2.13	0.49
1:C:545:ARG:HD2	1:C:716:SER:O	2.12	0.49
1:D:533:ARG:CG	1:D:533:ARG:HH11	2.25	0.49
1:D:628:LYS:CG	1:D:631:LYS:HD2	2.42	0.49
1:D:502:GLU:O	1:D:505:LYS:N	2.46	0.49
1:C:509:GLN:HA	1:C:509:GLN:NE2	2.28	0.49
1:D:498:LEU:O	1:D:498:LEU:CD1	2.52	0.49
1:B:644:LEU:HA	1:B:658:LEU:HD23	1.94	0.49
1:C:503:MET:O	1:C:504:GLU:C	2.50	0.49
1:C:542:ASN:N	1:C:542:ASN:HD22	2.11	0.49
1:D:752:GLU:O	1:D:755:LYS:HB2	2.12	0.49
1:B:576:GLU:HG2	1:B:734:LEU:CD2	2.43	0.49
1:D:508:GLU:OE1	1:D:512:LYS:HG3	2.12	0.48
1:A:542:ASN:N	1:A:542:ASN:HD22	2.11	0.48
1:A:741:PRO:O	1:A:744:VAL:HG23	2.12	0.48
1:C:503:MET:C	1:C:505:LYS:N	2.62	0.48
1:C:584:THR:O	1:C:714:HIS:HB2	2.14	0.48
1:A:547:ARG:HD3	2:A:802:BGD:O34	2.12	0.48
1:C:631:LYS:O	1:C:632:GLU:O	2.31	0.48
1:D:715:CYS:SG	1:D:718:GLY:HA2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:PHE:HA	3:A:3046:HOH:O	2.12	0.48
1:C:523:ILE:HD11	1:C:747:LYS:CD	2.43	0.48
3:B:3334:HOH:O	1:C:699:ARG:HG2	2.11	0.48
1:A:633:MET:CE	1:A:642:LEU:HD23	2.44	0.48
1:B:542:ASN:HD22	1:B:542:ASN:N	2.11	0.48
1:D:612:ARG:HG2	3:D:3451:HOH:O	2.13	0.48
1:B:620:LYS:NZ	3:B:3316:HOH:O	2.43	0.48
1:C:591:THR:O	1:C:591:THR:CG2	2.61	0.48
1:A:557:ILE:HD11	1:A:571:LEU:HB2	1.94	0.48
1:A:657:GLN:NE2	1:A:670:GLU:OE2	2.46	0.48
1:C:630:GLU:C	1:C:632:GLU:N	2.65	0.48
1:C:557:ILE:HD11	1:C:571:LEU:HB2	1.96	0.48
1:C:684:VAL:CG2	3:C:3191:HOH:O	2.62	0.48
1:D:691:PHE:O	1:D:694:PHE:HB3	2.14	0.48
1:C:533:ARG:HG3	1:C:533:ARG:NH1	2.21	0.47
1:D:652:TYR:CD2	1:D:690:SER:HB2	2.49	0.47
1:A:691:PHE:O	1:A:694:PHE:HB3	2.14	0.47
1:C:628:LYS:O	1:C:631:LYS:N	2.47	0.47
1:C:530:PHE:HB3	1:C:531:PRO:HD2	1.96	0.47
1:A:509:GLN:HA	1:A:509:GLN:NE2	2.28	0.47
1:A:615:GLU:HB2	1:A:620:LYS:HG2	1.96	0.47
1:B:499:GLU:CB	1:B:502:GLU:OE2	2.62	0.47
1:C:533:ARG:CG	1:C:533:ARG:HH11	2.23	0.47
1:D:546:TYR:CD2	2:D:805:BGD:H382	2.50	0.47
1:B:519:ILE:HA	1:B:522:ASP:OD2	2.14	0.47
1:C:666:GLN:NE2	3:C:3353:HOH:O	2.47	0.47
1:B:497:LYS:O	1:B:782:MET:HE1	2.14	0.47
1:C:650:LYS:HE2	3:C:3472:HOH:O	2.13	0.47
1:C:519:ILE:O	1:C:523:ILE:HD12	2.14	0.47
1:D:547:ARG:HA	3:D:3367:HOH:O	2.14	0.47
1:B:732:LEU:HA	1:B:732:LEU:HD23	1.80	0.46
1:A:775:ILE:O	1:A:778:ALA:HB3	2.16	0.46
1:D:645:ILE:HD11	1:D:659:GLU:HB2	1.96	0.46
1:B:576:GLU:HG2	1:B:734:LEU:HD21	1.97	0.46
1:D:615:GLU:HB2	1:D:620:LYS:CG	2.43	0.46
1:D:760:LEU:O	1:D:761:ILE:HB	2.16	0.46
1:A:503:MET:HE2	1:A:742:SER:HA	1.97	0.46
1:A:783:GLY:HA2	1:D:693:ASN:CG	2.35	0.46
1:B:670:GLU:HG3	3:B:3141:HOH:O	2.15	0.46
1:C:702:GLY:O	1:C:705:SER:HB3	2.16	0.46
1:C:546:TYR:CG	2:C:804:BGD:H382	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:THR:HG23	1:B:591:THR:O	2.16	0.46
1:C:517:ALA:O	1:C:521:GLN:NE2	2.49	0.46
1:D:547:ARG:HD2	2:D:805:BGD:H27	1.98	0.46
1:B:508:GLU:OE1	1:B:508:GLU:HA	2.16	0.45
1:B:781:ILE:C	1:B:783:GLY:H	2.19	0.45
1:C:775:ILE:O	1:C:778:ALA:HB3	2.16	0.45
1:D:503:MET:O	1:D:775:ILE:HD11	2.16	0.45
1:C:606:GLY:O	1:C:711:VAL:HG23	2.17	0.45
1:C:631:LYS:HA	1:C:631:LYS:HD2	1.52	0.45
1:B:735:MET:HG2	1:B:744:VAL:HG21	1.98	0.45
1:C:526:GLU:O	3:C:3470:HOH:O	2.21	0.45
1:B:665:THR:O	1:B:666:GLN:HB2	2.15	0.45
1:D:505:LYS:HG3	3:D:3271:HOH:O	2.17	0.45
1:D:628:LYS:HG3	1:D:631:LYS:HB2	1.99	0.45
1:C:539:LYS:HE3	3:C:3294:HOH:O	2.17	0.45
1:D:520:TYR:CE2	1:D:524:ARG:HD3	2.52	0.45
1:B:500:PHE:HZ	1:B:779:LYS:NZ	2.14	0.45
1:C:547:ARG:HE	1:C:547:ARG:HB3	1.58	0.45
1:C:647:GLU:HB3	3:C:3207:HOH:O	2.17	0.45
1:C:760:LEU:O	1:C:761:ILE:HB	2.17	0.45
1:D:657:GLN:NE2	1:D:670:GLU:OE2	2.49	0.45
1:A:661:GLU:HB2	1:A:668:THR:HG22	1.99	0.45
1:C:576:GLU:HG2	1:C:734:LEU:HD21	1.99	0.45
1:D:774:VAL:O	1:D:778:ALA:HB2	2.17	0.45
1:B:499:GLU:CG	1:B:502:GLU:OE2	2.65	0.44
1:C:685:PRO:HD2	1:C:769:PHE:CD2	2.52	0.44
1:D:661:GLU:HB2	1:D:668:THR:CG2	2.48	0.44
1:D:575:GLU:O	1:D:576:GLU:C	2.55	0.44
1:D:746:ILE:HG13	1:D:771:TYR:CD1	2.52	0.44
1:C:591:THR:O	1:C:591:THR:HG23	2.17	0.44
1:B:685:PRO:HD2	1:B:769:PHE:CE1	2.52	0.44
1:C:661:GLU:HG3	1:C:668:THR:HG23	1.99	0.44
1:C:746:ILE:HG13	1:C:771:TYR:CE2	2.53	0.44
1:B:579:ARG:CZ	1:B:733:LEU:HD11	2.48	0.44
1:D:770:SER:O	1:D:771:TYR:C	2.55	0.44
1:B:629:GLU:C	1:B:631:LYS:N	2.72	0.44
1:A:742:SER:C	1:A:744:VAL:H	2.21	0.43
1:B:774:VAL:O	1:B:778:ALA:HB2	2.18	0.43
1:D:544:ASN:OD1	1:D:568:ASN:ND2	2.45	0.43
1:A:648:ASP:OD2	1:A:650:LYS:NZ	2.49	0.43
1:C:730:THR:O	1:C:733:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:GLU:O	1:D:505:LYS:HB3	2.17	0.43
1:D:646:SER:H	1:D:657:GLN:HB3	1.82	0.43
1:D:681:ASP:HA	1:D:721:ARG:CZ	2.48	0.43
1:D:685:PRO:HD2	1:D:769:PHE:CE2	2.54	0.43
1:A:653:TYR:CD1	1:A:653:TYR:C	2.92	0.43
1:C:513:SER:O	1:C:514:GLY:C	2.57	0.43
1:C:775:ILE:HG22	1:C:776:GLU:N	2.33	0.43
1:D:731:CYS:O	1:D:735:MET:HG3	2.18	0.43
1:A:648:ASP:OD2	1:A:650:LYS:HE2	2.18	0.43
1:A:681:ASP:O	1:A:682:PHE:HB2	2.18	0.43
1:B:697:LYS:HE2	3:B:3386:HOH:O	2.18	0.43
1:B:528:SER:HB3	1:B:530:PHE:CE1	2.53	0.43
1:B:650:LYS:HD2	1:B:653:TYR:CE1	2.54	0.43
1:B:775:ILE:HG22	1:B:776:GLU:N	2.34	0.43
1:C:738:ARG:HH11	1:C:744:VAL:HA	1.84	0.43
1:A:742:SER:O	1:A:744:VAL:N	2.52	0.43
1:B:549:VAL:HG21	1:B:717:ALA:HB1	2.01	0.43
1:A:523:ILE:HG13	1:A:747:LYS:HD2	2.01	0.43
1:A:781:ILE:C	1:A:783:GLY:H	2.22	0.43
1:C:502:GLU:CG	1:C:503:MET:N	2.82	0.43
1:B:499:GLU:OE1	1:B:740:ASP:OD1	2.37	0.43
1:C:507:PHE:CE2	1:C:516:TRP:HZ2	2.36	0.43
1:D:500:PHE:O	1:D:501:MET:C	2.57	0.43
1:D:611:ASN:HD21	1:D:621:CYS:HB2	1.84	0.43
1:A:647:GLU:HG2	1:A:649:ILE:HD11	2.01	0.42
1:B:691:PHE:O	1:B:694:PHE:HB3	2.19	0.42
1:B:584:THR:O	1:B:714:HIS:HB2	2.19	0.42
1:B:657:GLN:NE2	1:B:670:GLU:OE2	2.52	0.42
1:C:542:ASN:HD22	1:C:542:ASN:H	1.66	0.42
1:D:699:ARG:HA	1:D:704:LEU:HD12	2.01	0.42
1:A:547:ARG:HD2	2:A:802:BGD:C4	2.48	0.42
1:A:626:PRO:HB3	1:A:631:LYS:HB3	2.01	0.42
1:A:696:PHE:CD1	1:A:696:PHE:N	2.87	0.42
1:B:611:ASN:HD21	1:B:621:CYS:HB2	1.85	0.42
1:C:576:GLU:HG2	1:C:734:LEU:CD2	2.49	0.42
1:B:543:ARG:HD3	3:B:3096:HOH:O	2.19	0.42
1:C:508:GLU:OE1	1:C:508:GLU:HA	2.15	0.42
1:C:720:GLY:N	2:C:804:BGD:O50	2.40	0.42
1:A:783:GLY:HA2	1:D:693:ASN:OD1	2.19	0.42
1:D:752:GLU:HA	1:D:755:LYS:CE	2.46	0.42
1:A:627:GLN:H	1:A:631:LYS:CD	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:LYS:HA	1:B:536:LYS:HD3	1.84	0.42
1:B:760:LEU:O	1:B:761:ILE:HB	2.19	0.42
1:D:628:LYS:NZ	1:D:631:LYS:HD2	2.34	0.42
1:A:592:CYS:HB2	3:A:3070:HOH:O	2.18	0.42
1:B:676:TYR:CD2	1:B:679:TRP:HB2	2.55	0.42
1:C:533:ARG:CG	1:C:533:ARG:NH1	2.81	0.42
1:C:615:GLU:HB2	1:C:620:LYS:CG	2.44	0.42
1:C:740:ASP:HA	1:C:741:PRO:HD2	1.87	0.42
1:D:533:ARG:HG3	1:D:533:ARG:NH1	2.27	0.42
1:A:730:THR:O	1:A:733:LEU:HB2	2.20	0.42
1:A:533:ARG:NH1	1:A:533:ARG:CG	2.80	0.42
1:C:539:LYS:H	1:C:539:LYS:HG2	1.64	0.42
1:D:500:PHE:O	1:D:502:GLU:N	2.53	0.42
1:D:775:ILE:HG22	1:D:776:GLU:N	2.34	0.42
1:A:760:LEU:O	1:A:761:ILE:HB	2.19	0.41
1:B:649:ILE:HG12	1:B:654:THR:CG2	2.49	0.41
1:C:502:GLU:CD	1:C:742:SER:HB3	2.39	0.41
1:C:781:ILE:C	1:C:783:GLY:H	2.23	0.41
1:D:778:ALA:O	1:D:782:MET:HG2	2.20	0.41
1:A:652:TYR:HA	1:A:678:THR:HG23	2.01	0.41
1:C:661:GLU:HB2	1:C:668:THR:HG22	2.01	0.41
1:B:707:GLU:CD	1:C:708:HIS:CE1	2.93	0.41
1:A:629:GLU:HA	1:A:644:LEU:HD23	2.02	0.41
1:A:661:GLU:HG3	1:A:668:THR:HG23	2.01	0.41
1:D:609:MET:HG3	1:D:714:HIS:CE1	2.54	0.41
1:C:609:MET:HG3	1:C:714:HIS:CE1	2.56	0.41
1:A:626:PRO:HA	1:A:631:LYS:HD3	2.02	0.41
1:A:633:MET:HE3	1:A:635:PHE:HZ	1.85	0.41
1:C:536:LYS:HA	1:C:536:LYS:HD3	1.84	0.41
1:D:545:ARG:HG3	1:D:545:ARG:NH1	2.34	0.41
1:A:508:GLU:HA	1:A:508:GLU:OE1	2.20	0.41
1:A:542:ASN:HD22	1:A:542:ASN:H	1.67	0.41
1:A:692:LEU:O	1:A:696:PHE:CD1	2.73	0.41
1:A:530:PHE:HB3	1:A:531:PRO:HD2	2.01	0.41
1:A:647:GLU:HG2	1:A:649:ILE:CD1	2.51	0.41
1:D:661:GLU:HG3	1:D:668:THR:HG23	2.03	0.41
1:D:775:ILE:O	1:D:778:ALA:HB3	2.20	0.41
1:C:515:SER:O	1:C:519:ILE:HG13	2.20	0.41
1:A:633:MET:CE	1:A:635:PHE:HZ	2.34	0.41
1:D:533:ARG:CG	1:D:533:ARG:NH1	2.82	0.41
1:D:547:ARG:HH21	2:D:805:BGD:C5	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:781:ILE:C	1:D:783:GLY:H	2.24	0.41
1:A:515:SER:O	1:A:519:ILE:HG13	2.21	0.41
1:A:528:SER:HB3	1:A:530:PHE:CE1	2.56	0.41
1:C:679:TRP:NE1	1:C:721:ARG:HG2	2.35	0.41
1:D:530:PHE:HB3	1:D:531:PRO:HD2	2.02	0.41
1:D:542:ASN:N	1:D:542:ASN:ND2	2.67	0.41
1:D:628:LYS:O	1:D:628:LYS:HG3	2.21	0.41
1:D:628:LYS:CD	1:D:631:LYS:HD2	2.51	0.41
1:B:626:PRO:HB2	1:B:644:LEU:HB2	2.03	0.40
1:A:536:LYS:HA	1:A:536:LYS:HD3	1.85	0.40
1:A:679:TRP:NE1	1:A:721:ARG:HG2	2.37	0.40
1:B:619:LEU:N	1:B:619:LEU:HD12	2.36	0.40
1:C:665:THR:C	3:C:3292:HOH:O	2.59	0.40
1:D:646:SER:OG	1:D:657:GLN:HB2	2.22	0.40
1:A:575:GLU:O	1:A:578:GLN:N	2.54	0.40
1:A:652:TYR:HA	1:A:678:THR:CG2	2.51	0.40
1:A:685:PRO:HD2	1:A:769:PHE:CD2	2.56	0.40
1:B:542:ASN:HD22	1:B:542:ASN:H	1.69	0.40
1:B:715:CYS:SG	1:B:718:GLY:HA2	2.60	0.40
1:B:719:ILE:HG13	1:B:720:GLY:N	2.37	0.40
1:C:537:LEU:CD1	1:C:537:LEU:N	2.85	0.40
1:C:735:MET:HG2	1:C:744:VAL:HG21	2.03	0.40
1:A:715:CYS:SG	1:A:718:GLY:HA2	2.61	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	285/295 (97%)	255 (90%)	27 (10%)	3 (1%)	17 29
1	B	285/295 (97%)	262 (92%)	18 (6%)	5 (2%)	10 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	285/295 (97%)	260 (91%)	21 (7%)	4 (1%)	13	23
1	D	285/295 (97%)	252 (88%)	28 (10%)	5 (2%)	10	17
All	All	1140/1180 (97%)	1029 (90%)	94 (8%)	17 (2%)	12	21

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	629	GLU
1	B	629	GLU
1	C	632	GLU
1	C	651	SER
1	D	575	GLU
1	A	743	SER
1	B	498	LEU
1	B	630	GLU
1	B	575	GLU
1	C	761	ILE
1	D	563	ASP
1	D	647	GLU
1	D	761	ILE
1	A	761	ILE
1	B	761	ILE
1	C	630	GLU
1	D	503	MET

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	257/268 (96%)	244 (95%)	13 (5%)	28	50
1	B	257/268 (96%)	242 (94%)	15 (6%)	23	43
1	C	254/268 (95%)	238 (94%)	16 (6%)	21	38
1	D	258/268 (96%)	249 (96%)	9 (4%)	41	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1026/1072 (96%)	973 (95%)	53 (5%)	27 49

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	497	LYS
1	A	508	GLU
1	A	511	ASP
1	A	522	ASP
1	A	537	LEU
1	A	542	ASN
1	A	591	THR
1	A	605	ARG
1	A	614	MET
1	A	619	LEU
1	A	636	GLU
1	A	668	THR
1	A	715	CYS
1	B	508	GLU
1	B	511	ASP
1	B	521	GLN
1	B	537	LEU
1	B	542	ASN
1	B	547	ARG
1	B	591	THR
1	B	605	ARG
1	B	612	ARG
1	B	628	LYS
1	B	632	GLU
1	B	636	GLU
1	B	668	THR
1	B	715	CYS
1	B	755	LYS
1	C	502	GLU
1	C	503	MET
1	C	511	ASP
1	C	521	GLN
1	C	522	ASP
1	C	537	LEU
1	C	542	ASN
1	C	548	ASP
1	C	591	THR

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Mol	Chain	Res	Type
1	C	636	GLU
1	C	651	SER
1	C	668	THR
1	C	700	GLU
1	C	715	CYS
1	C	742	SER
1	C	772	LEU
1	D	508	GLU
1	D	511	ASP
1	D	537	LEU
1	D	542	ASN
1	D	591	THR
1	D	613	VAL
1	D	614	MET
1	D	631	LYS
1	D	636	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	509	GLN
1	A	521	GLN
1	A	542	ASN
1	A	594	HIS
1	B	509	GLN
1	B	542	ASN
1	B	627	GLN
1	B	657	GLN
1	B	666	GLN
1	C	509	GLN
1	C	542	ASN
1	C	666	GLN
1	C	693	ASN
1	D	540	ASN
1	D	542	ASN
1	D	560	HIS
1	D	561	GLN
1	D	564	ASN
1	D	594	HIS
1	D	657	GLN
1	D	666	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	BGD	A	802	-	45,56,56	3.47	26 (57%)	65,83,83	1.19	7 (10%)
2	BGD	B	803	-	45,56,56	3.32	23 (51%)	65,83,83	1.43	13 (20%)
2	BGD	C	804	-	45,56,56	3.34	26 (57%)	65,83,83	1.17	6 (9%)
2	BGD	D	805	-	45,56,56	3.35	24 (53%)	65,83,83	1.36	9 (13%)

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	BGD	A	802	-	-	0/59/71/71	0/3/3/3
2	BGD	B	803	-	-	0/59/71/71	0/3/3/3
2	BGD	C	804	-	-	0/59/71/71	0/3/3/3
2	BGD	D	805	-	-	0/59/71/71	0/3/3/3

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	804	BGD	C52-N54	-5.11	1.23	1.32
2	A	802	BGD	C52-N54	-5.00	1.23	1.32
2	D	805	BGD	C52-N54	-3.77	1.25	1.32
2	B	803	BGD	C52-N54	-3.03	1.27	1.32
2	D	805	BGD	P32-O34	2.06	1.58	1.54
2	C	804	BGD	C40-C39	2.08	1.43	1.38
2	B	803	BGD	C40-C39	2.08	1.43	1.38
2	C	804	BGD	O53-C52	2.09	1.27	1.23
2	A	802	BGD	P32-O35	2.09	1.58	1.54
2	C	804	BGD	C38-C37	2.10	1.59	1.54
2	A	802	BGD	C19-N18	2.10	1.50	1.45
2	A	802	BGD	C38-C37	2.12	1.59	1.54
2	D	805	BGD	C37-C52	2.18	1.57	1.52
2	A	802	BGD	C37-N36	2.18	1.50	1.45
2	C	804	BGD	P32-O35	2.21	1.58	1.54
2	C	804	BGD	C17-N16	2.43	1.51	1.45
2	D	805	BGD	P32-O35	2.46	1.59	1.54
2	B	803	BGD	O53-C52	2.46	1.28	1.23
2	A	802	BGD	P48-O49	2.57	1.54	1.50
2	A	802	BGD	C37-C52	2.67	1.58	1.52
2	B	803	BGD	P48-O49	2.79	1.54	1.50
2	C	804	BGD	C37-C52	2.91	1.59	1.52
2	B	803	BGD	C41-C40	2.93	1.44	1.38
2	D	805	BGD	C17-N16	3.07	1.52	1.45
2	C	804	BGD	P48-O49	3.17	1.55	1.50
2	D	805	BGD	C24-C23	3.34	1.45	1.38
2	A	802	BGD	C17-N16	3.46	1.53	1.45
2	B	803	BGD	C37-C52	3.53	1.60	1.52
2	A	802	BGD	C25-C24	3.59	1.45	1.38
2	C	804	BGD	C15-C14	3.61	1.46	1.38
2	C	804	BGD	C15-C13	3.62	1.46	1.38
2	B	803	BGD	C15-C13	3.66	1.46	1.38
2	A	802	BGD	C24-C23	3.66	1.46	1.38
2	D	805	BGD	C15-C13	3.75	1.47	1.38
2	B	803	BGD	C24-C23	3.81	1.46	1.38
2	D	805	BGD	C25-C24	3.82	1.45	1.38
2	A	802	BGD	C42-C39	3.86	1.46	1.38
2	D	805	BGD	C27-C26	3.93	1.45	1.38
2	B	803	BGD	C26-C23	3.94	1.47	1.38
2	A	802	BGD	C15-C13	3.94	1.47	1.38
2	D	805	BGD	C15-C14	3.94	1.47	1.38
2	C	804	BGD	C26-C23	3.98	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	BGD	C15-C14	4.01	1.47	1.38
2	C	804	BGD	C14-C12	4.04	1.46	1.38
2	D	805	BGD	C41-C40	4.09	1.46	1.38
2	C	804	BGD	C27-C26	4.10	1.46	1.38
2	B	803	BGD	C15-C14	4.10	1.48	1.38
2	A	802	BGD	C43-C44	4.12	1.45	1.39
2	C	804	BGD	C13-C11	4.15	1.46	1.38
2	D	805	BGD	P48-O49	4.17	1.57	1.50
2	C	804	BGD	C41-C40	4.18	1.46	1.38
2	A	802	BGD	C27-C26	4.19	1.46	1.38
2	C	804	BGD	C24-C23	4.22	1.47	1.38
2	C	804	BGD	C25-C24	4.22	1.46	1.38
2	B	803	BGD	C14-C12	4.28	1.47	1.38
2	D	805	BGD	C42-C39	4.32	1.47	1.38
2	B	803	BGD	C12-C10	4.38	1.46	1.39
2	C	804	BGD	C42-C39	4.39	1.48	1.38
2	B	803	BGD	C25-C24	4.41	1.46	1.38
2	B	803	BGD	C42-C39	4.41	1.48	1.38
2	B	803	BGD	C13-C11	4.43	1.47	1.38
2	D	805	BGD	C26-C23	4.48	1.48	1.38
2	D	805	BGD	C14-C12	4.50	1.47	1.38
2	C	804	BGD	C43-C42	4.63	1.47	1.38
2	A	802	BGD	C26-C23	4.64	1.48	1.38
2	D	805	BGD	C41-C44	4.71	1.46	1.39
2	D	805	BGD	C13-C11	4.73	1.47	1.38
2	B	803	BGD	C41-C44	4.78	1.47	1.39
2	A	802	BGD	C14-C12	4.86	1.48	1.38
2	A	802	BGD	C13-C11	4.92	1.48	1.38
2	B	803	BGD	P32-O33	5.07	1.58	1.50
2	B	803	BGD	C27-C26	5.08	1.47	1.38
2	C	804	BGD	C12-C10	5.16	1.47	1.39
2	A	802	BGD	C41-C40	5.17	1.48	1.38
2	A	802	BGD	P32-O33	5.26	1.58	1.50
2	B	803	BGD	C43-C42	5.26	1.48	1.38
2	C	804	BGD	P32-O33	5.30	1.59	1.50
2	C	804	BGD	C43-C44	5.37	1.47	1.39
2	B	803	BGD	C25-C28	5.41	1.48	1.39
2	A	802	BGD	C25-C28	5.42	1.48	1.39
2	D	805	BGD	P32-O33	5.47	1.59	1.50
2	D	805	BGD	C43-C42	5.49	1.48	1.38
2	A	802	BGD	C43-C42	5.54	1.48	1.38
2	C	804	BGD	C11-C10	5.55	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	BGD	C12-C10	5.58	1.48	1.39
2	D	805	BGD	C25-C28	5.66	1.48	1.39
2	D	805	BGD	C12-C10	5.72	1.48	1.39
2	D	805	BGD	C27-C28	5.85	1.48	1.39
2	D	805	BGD	C43-C44	5.93	1.48	1.39
2	C	804	BGD	C41-C44	5.96	1.48	1.39
2	D	805	BGD	C11-C10	6.08	1.49	1.39
2	B	803	BGD	C43-C44	6.10	1.49	1.39
2	C	804	BGD	C25-C28	6.15	1.49	1.39
2	C	804	BGD	C27-C28	6.15	1.49	1.39
2	A	802	BGD	C41-C44	6.18	1.49	1.39
2	A	802	BGD	C11-C10	6.45	1.50	1.39
2	B	803	BGD	C11-C10	6.53	1.50	1.39
2	A	802	BGD	C27-C28	6.71	1.50	1.39
2	B	803	BGD	C27-C28	7.02	1.50	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	805	BGD	F30-C29-C28	-3.21	105.84	110.46
2	B	803	BGD	C1-C17-N16	-2.98	103.00	111.20
2	C	804	BGD	F47-C45-C44	-2.90	106.27	110.46
2	B	803	BGD	O9-C8-N16	-2.84	117.27	122.46
2	D	805	BGD	O50-P48-O49	-2.79	106.81	113.05
2	A	802	BGD	O34-P32-O33	-2.75	106.89	113.05
2	D	805	BGD	C38-C37-N36	-2.74	104.99	110.80
2	D	805	BGD	C20-C19-N18	-2.70	103.77	111.20
2	D	805	BGD	O34-P32-O33	-2.68	107.05	113.05
2	B	803	BGD	O51-P48-O49	-2.66	107.09	113.05
2	B	803	BGD	O50-P48-O49	-2.63	107.16	113.05
2	A	802	BGD	O51-P48-O49	-2.54	107.37	113.05
2	B	803	BGD	F47-C45-C44	-2.45	106.92	110.46
2	C	804	BGD	C20-C19-N18	-2.37	104.68	111.20
2	C	804	BGD	O34-P32-O33	-2.37	107.75	113.05
2	B	803	BGD	O34-P32-O33	-2.36	107.77	113.05
2	B	803	BGD	C38-C39-C40	-2.23	116.41	120.91
2	B	803	BGD	C17-N16-C8	-2.22	115.83	121.56
2	B	803	BGD	O35-P32-O33	-2.18	108.18	113.05
2	A	802	BGD	F47-C45-C44	-2.14	107.38	110.46
2	B	803	BGD	C22-C19-C20	-2.07	104.68	110.28
2	C	804	BGD	O50-P48-O49	-2.04	108.49	113.05
2	A	802	BGD	O9-C8-N16	-2.01	118.79	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	BGD	C19-C20-N36	2.01	121.32	116.78
2	D	805	BGD	C19-N18-C1	2.28	126.66	121.66
2	B	803	BGD	P48-C45-C44	2.30	115.86	108.95
2	D	805	BGD	C39-C38-C37	2.58	120.61	113.41
2	D	805	BGD	C10-C8-N16	2.61	121.78	116.97
2	A	802	BGD	P32-C29-C28	2.66	116.94	108.95
2	B	803	BGD	P32-C29-C28	2.99	117.93	108.95
2	A	802	BGD	C10-C8-N16	3.09	122.67	116.97
2	C	804	BGD	P48-C45-C44	3.20	118.55	108.95
2	C	804	BGD	P32-C29-C28	3.49	119.43	108.95
2	B	803	BGD	C10-C8-N16	3.65	123.71	116.97
2	D	805	BGD	P32-C29-C28	4.04	121.09	108.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	BGD	6	0
2	B	803	BGD	2	0
2	C	804	BGD	5	0
2	D	805	BGD	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	287/295 (97%)	-0.11	9 (3%)	49	52	13, 37, 71, 100	0
1	B	287/295 (97%)	-0.27	2 (0%)	87	88	9, 27, 64, 92	0
1	C	287/295 (97%)	0.05	17 (5%)	23	24	13, 37, 84, 100	0
1	D	287/295 (97%)	0.28	13 (4%)	34	36	22, 54, 83, 100	0
All	All	1148/1180 (97%)	-0.01	41 (3%)	43	45	9, 38, 80, 100	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	782	MET	7.6
1	B	781	ILE	4.8
1	D	630	GLU	4.5
1	A	781	ILE	4.4
1	A	783	GLY	4.3
1	D	629	GLU	4.1
1	C	498	LEU	4.0
1	D	541	LYS	3.7
1	A	630	GLU	3.6
1	A	782	MET	3.6
1	C	512	LYS	3.5
1	C	630	GLU	3.5
1	C	509	GLN	3.4
1	D	664	THR	3.3
1	A	616	LYS	3.3
1	C	783	GLY	3.1
1	D	780	PHE	3.1
1	B	782	MET	2.9
1	C	510	ILE	2.9
1	D	783	GLY	2.7
1	D	614	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	502	GLU	2.6
1	C	505	LYS	2.5
1	C	529	ASP	2.5
1	C	501	MET	2.5
1	A	629	GLU	2.5
1	D	628	LYS	2.4
1	D	634	ILE	2.4
1	C	771	TYR	2.4
1	D	658	LEU	2.4
1	C	682	PHE	2.4
1	D	538	PRO	2.3
1	C	629	GLU	2.2
1	C	500	PHE	2.2
1	A	512	LYS	2.2
1	C	515	SER	2.2
1	C	499	GLU	2.2
1	A	500	PHE	2.2
1	A	736	ASP	2.1
1	D	536	LYS	2.1
1	D	535	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	BGD	A	802	54/54	0.87	0.23	2.96	36,75,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BGD	B	803	54/54	0.93	0.17	1.41	13,50,68,70	0
2	BGD	D	805	54/54	0.83	0.22	1.18	41,72,100,100	0
2	BGD	C	804	54/54	0.82	0.21	1.03	42,78,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.