



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:56 AM UTC

PDB ID : 1EWT / pdb_00001ewt
Title : CRYSTAL STRUCTURE OF METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1 LIGAND FREE FORM I
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Deposited on : 2000-04-27
Resolution : 3.70 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

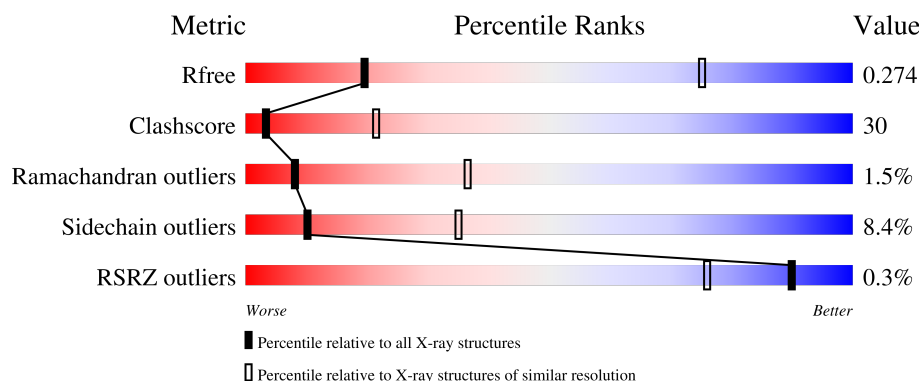
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	490	
1	B	490	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7282 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 METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3624	2297	632	675	20			
1	B	456	Total	C	N	O	S	0	0	0
			3624	2297	632	675	20			

- 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	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	14	8	1	5	0	0

3509	C439	N362	R285	F201
YS10	D440	N365	V286	L202
YS11	A441	P366	V287	R203
IS12	M442	V288	V288	V204
GLN		C289	C289	V205
MET	I445	F368	F290	P206
ASN	D446	P369	C291	S207
LYS	G447	E370	E292	D208
SER	R448	F371	G293	T209
GLY	K449	W372	M294	L210
MET	K450	Q373	T295	Q211
VAL	L451	H374	V296	A212
ARG	D452	R375	R297	R213
SER	F453	F376	G298	A214
	L454	Q377	L299	M215
		C378	L300	
	S457	R379	S301	I218
	S458	L380	A302	V219
	F459		M303	K220
	V460	L384	R304	R221
	G461	L395	R305	Y222
	V462	E386	L306	N223
	S463	N387	G307	W224
	G464	P388		
	E465	M389	F312	V227
	E466	F390	S313	S228
	V467		L314	A229
		C394		V230
	A475	T395	S317	H231
	P476	G396	D318	T232
	G477	N397	G319	E233
	R478	E398	W320	
	Y479	S399		Y236
	D480	L400	R323	G237
	I481	E401	D324	M241
	M482		E325	D242
	N483			A243
	L484			F244
	Q485			E246
	Y486			L247
	T487			
	E488			L253
	A489			
	N490			A256
	R491	A419	E331	H257
	Y492	M420	V332	
	D493	A421	E333	I261
	Y494		A334	Y262
	Y495	H422	G336	
	H496	G423		
	V497	L424	T339	I261
		Q425	K341	
		H426	L342	
		M427	Q343	F270
	W500	H428		
	H501		Y353	L273
	E502		F354	
			L355	R278
	L505		K356	E279
	M506		L357	R280
	T507		R358	
	D508			A284

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.44Å 111.44Å 293.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.70 12.00 – 3.71	Depositor EDS
% Data completeness (in resolution range)	99.7 (12.00-3.70) 96.2 (12.00-3.71)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 3.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.287 0.233 , 0.274	Depositor DCC
R_{free} test set	950 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	92.5	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7282	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: NAG, 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	0.86	4/3704 (0.1%)	1.27	25/5009 (0.5%)
1	B	0.86	4/3704 (0.1%)	1.28	21/5009 (0.4%)
All	All	0.86	8/7408 (0.1%)	1.28	46/10018 (0.5%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	TRP	NE1-CE2	10.45	1.49	1.37
1	B	500	TRP	NE1-CE2	10.42	1.49	1.37
1	A	500	TRP	NE1-CE2	10.37	1.48	1.37
1	A	224	TRP	NE1-CE2	10.35	1.48	1.37
1	A	110	TRP	NE1-CE2	10.24	1.48	1.37
1	A	367	TRP	NE1-CE2	10.21	1.48	1.37
1	B	110	TRP	NE1-CE2	10.19	1.48	1.37
1	B	367	TRP	NE1-CE2	8.54	1.46	1.37

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	ILE	O-C-N	-8.85	115.80	121.37
1	A	130	ILE	N-CA-C	-8.14	105.25	113.47
1	B	380	LEU	CA-C-N	7.49	129.20	119.84
1	B	380	LEU	C-N-CA	7.49	129.20	119.84
1	A	204	VAL	N-CA-C	-7.36	104.34	112.80
1	B	398	GLU	N-CA-C	-6.89	101.44	110.53
1	B	154	LYS	CA-C-N	6.53	126.71	120.31
1	B	154	LYS	C-N-CA	6.53	126.71	120.31
1	A	159	VAL	N-CA-C	5.90	116.61	108.12
1	A	324	ASP	O-C-N	5.88	129.10	122.22
1	B	159	VAL	N-CA-C	5.80	116.47	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	LYS	N-CA-C	-5.77	101.92	110.46
1	B	319	GLY	N-CA-C	-5.74	105.42	112.77
1	A	154	LYS	CA-C-N	5.71	125.91	120.31
1	A	154	LYS	C-N-CA	5.71	125.91	120.31
1	B	292	GLU	N-CA-C	-5.67	103.43	110.41
1	A	395	THR	N-CA-C	-5.66	105.09	112.23
1	A	364	ARG	N-CA-C	5.64	119.89	112.89
1	B	475	ALA	CA-C-N	5.62	125.53	119.85
1	B	475	ALA	C-N-CA	5.62	125.53	119.85
1	A	319	GLY	N-CA-C	-5.61	105.59	112.77
1	A	452	ASP	CA-CB-CG	-5.48	107.12	112.60
1	B	476	PRO	CA-C-N	5.46	125.87	120.31
1	B	476	PRO	C-N-CA	5.46	125.87	120.31
1	B	395	THR	N-CA-C	-5.41	105.94	112.54
1	A	205	VAL	CA-C-N	5.39	125.68	119.92
1	A	205	VAL	C-N-CA	5.39	125.68	119.92
1	A	201	PHE	CA-CB-CG	-5.35	108.45	113.80
1	B	494	TYR	O-C-N	-5.33	116.25	122.96
1	A	208	ASP	CA-C-N	-5.31	113.17	120.28
1	A	208	ASP	C-N-CA	-5.31	113.17	120.28
1	B	478	ARG	CD-NE-CZ	-5.29	116.99	124.40
1	B	221	ARG	CD-NE-CZ	-5.28	117.00	124.40
1	A	290	PHE	CA-CB-CG	-5.23	108.57	113.80
1	A	221	ARG	CD-NE-CZ	-5.22	117.10	124.40
1	B	131	ARG	CD-NE-CZ	-5.19	117.13	124.40
1	A	218	ILE	N-CA-C	-5.18	105.49	110.72
1	A	65	ARG	CD-NE-CZ	-5.17	117.16	124.40
1	A	491	ARG	CD-NE-CZ	-5.15	117.19	124.40
1	B	40	ARG	CD-NE-CZ	-5.14	117.20	124.40
1	A	379	ARG	CD-NE-CZ	-5.14	117.21	124.40
1	A	163	GLY	O-C-N	-5.10	117.30	122.19
1	A	96	LEU	CA-C-N	5.09	126.21	119.84
1	A	96	LEU	C-N-CA	5.09	126.21	119.84
1	B	285	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	B	467	VAL	N-CA-C	5.09	115.45	108.12

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	3624	0	3553	224	0
1	B	3624	0	3552	221	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
3	B	14	0	13	1	0
All	All	7282	0	7118	435	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 30.

All (435) 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:427:MET:HE2	1:B:442:MET:HG2	1.36	1.04
1:A:362:ASN:HD21	1:A:365:ASN:HB3	1.22	1.00
1:A:278:ARG:HH11	1:A:306:LEU:HD21	1.28	0.98
1:B:278:ARG:HH11	1:B:306:LEU:HD21	1.29	0.97
1:B:407:ASP:HB3	1:B:410:MET:HB2	1.45	0.96
1:A:323:ARG:HB3	1:A:325:GLU:HG2	1.50	0.93
1:A:407:ASP:HB3	1:A:410:MET:HB2	1.49	0.93
1:B:323:ARG:HB3	1:B:325:GLU:HG2	1.50	0.91
1:A:82:MET:HE2	1:A:86:LEU:HD11	1.53	0.89
1:A:228:SER:HB2	1:A:287:VAL:HG22	1.54	0.89
1:A:218:ILE:HD11	1:A:481:ILE:HD12	1.51	0.89
1:B:218:ILE:HD11	1:B:481:ILE:HD12	1.56	0.88
1:B:82:MET:HE2	1:B:86:LEU:HD11	1.55	0.87
1:B:228:SER:HB2	1:B:287:VAL:HG22	1.55	0.87
1:B:461:GLY:HA3	1:B:465:GLU:HG3	1.57	0.86
1:B:257:HIS:HB2	1:B:280:ARG:HG3	1.57	0.85
1:B:300:LEU:CD2	1:B:334:ALA:HB2	2.09	0.83
1:A:162:PRO:HG3	1:A:171:VAL:HG21	1.61	0.82
1:A:39:ALA:HB3	1:A:105:ILE:HB	1.60	0.81
1:B:39:ALA:HB3	1:B:105:ILE:HB	1.62	0.81
1:A:257:HIS:HB2	1:A:280:ARG:HG3	1.62	0.80
1:B:205:VAL:HG23	1:B:206:PRO:HD2	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLY:O	1:A:159:VAL:HA	1.83	0.78
1:A:362:ASN:ND2	1:A:365:ASN:HB3	1.99	0.77
1:B:340:ILE:HG23	1:B:479:TYR:HB3	1.63	0.77
1:A:278:ARG:NH1	1:A:306:LEU:HD21	2.00	0.77
1:B:278:ARG:NH1	1:B:306:LEU:HD21	2.00	0.77
1:B:355:LEU:HD22	1:B:401:GLU:HG2	1.66	0.76
1:A:202:LEU:N	1:A:202:LEU:HD23	2.01	0.76
1:B:368:PHE:HB3	1:B:369:PRO:HD3	1.67	0.76
1:B:475:ALA:HB1	1:B:476:PRO:HD2	1.68	0.75
1:A:300:LEU:CD2	1:A:334:ALA:HB2	2.17	0.75
1:A:382:GLY:O	1:A:386:GLU:HB2	1.86	0.75
1:A:368:PHE:HB3	1:A:369:PRO:HD3	1.68	0.74
1:B:478:ARG:HG3	1:B:478:ARG:HH11	1.52	0.74
1:B:202:LEU:HD23	1:B:202:LEU:N	2.02	0.73
1:B:323:ARG:HB3	1:B:325:GLU:CG	2.18	0.73
1:B:423:GLY:HA3	1:B:454:LEU:HD23	1.70	0.73
1:B:73:GLN:HA	1:B:77:GLN:HE21	1.53	0.73
1:B:427:MET:CE	1:B:442:MET:HG2	2.16	0.73
1:B:98:ASN:CG	3:B:601:NAG:C1	2.59	0.73
1:A:73:GLN:HA	1:A:77:GLN:HE21	1.54	0.72
1:A:72:GLU:O	1:A:77:GLN:HG3	1.89	0.72
1:A:300:LEU:CD1	1:A:334:ALA:HB2	2.20	0.71
1:B:215:MET:O	1:B:219:VAL:HG23	1.91	0.71
1:A:334:ALA:O	1:A:484:LEU:HD23	1.91	0.71
1:B:358:ARG:HG2	1:B:358:ARG:HH11	1.56	0.71
1:B:205:VAL:CG2	1:B:206:PRO:HD2	2.21	0.70
1:A:230:VAL:O	1:A:289:CYS:HA	1.90	0.70
1:A:323:ARG:HB3	1:A:325:GLU:CG	2.21	0.70
1:B:89:ILE:HG21	1:B:101:LEU:HD12	1.72	0.70
1:B:300:LEU:HD22	1:B:334:ALA:HB2	1.74	0.70
1:A:227:VAL:HG12	1:A:286:VAL:HB	1.74	0.70
1:A:355:LEU:HD22	1:A:401:GLU:HG2	1.74	0.70
1:B:211:GLN:HA	1:B:479:TYR:CE1	2.28	0.69
1:A:383:HIS:CG	1:A:384:LEU:H	2.10	0.68
1:B:243:ALA:O	1:B:247:LEU:HB2	1.94	0.67
1:A:215:MET:O	1:A:219:VAL:HG23	1.95	0.67
1:A:427:MET:HE1	1:A:449:LYS:HB3	1.76	0.67
1:B:213:ARG:HH11	1:B:247:LEU:HD21	1.59	0.66
1:A:243:ALA:O	1:A:247:LEU:HB2	1.95	0.66
1:A:128:ILE:C	1:A:130:ILE:H	2.03	0.66
1:A:461:GLY:HA3	1:A:465:GLU:HG3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ASN:OD1	1:A:336:GLY:N	2.29	0.66
1:A:446:ASP:HB3	1:A:449:LYS:HD2	1.77	0.66
1:B:227:VAL:HG12	1:B:286:VAL:HB	1.78	0.66
1:A:303:MET:HE3	1:A:312:PHE:HD2	1.60	0.66
1:A:427:MET:HA	1:A:453:PHE:CZ	2.31	0.65
1:A:427:MET:HG2	1:A:442:MET:HE3	1.77	0.65
1:B:232:THR:HG21	1:B:292:GLU:OE2	1.97	0.65
1:B:278:ARG:HH11	1:B:306:LEU:CD2	2.07	0.65
1:A:461:GLY:N	1:A:465:GLU:O	2.28	0.65
1:A:169:ILE:HD11	1:A:192:LEU:HG	1.80	0.64
1:A:202:LEU:HD23	1:A:202:LEU:H	1.62	0.64
1:B:510:TYR:CD1	1:B:510:TYR:C	2.76	0.64
1:A:278:ARG:HH11	1:A:306:LEU:CD2	2.08	0.64
1:B:72:GLU:O	1:B:77:GLN:HG3	1.97	0.64
1:A:95:LEU:HD12	1:A:96:LEU:N	2.13	0.63
1:B:169:ILE:HD11	1:B:192:LEU:HG	1.80	0.63
1:B:202:LEU:HD23	1:B:202:LEU:H	1.62	0.63
1:B:228:SER:CB	1:B:287:VAL:HG22	2.28	0.63
1:A:154:LYS:HB2	1:A:154:LYS:NZ	2.12	0.63
1:B:297:ARG:HH12	1:B:328:GLU:HB3	1.62	0.63
1:A:402:GLU:O	1:A:403:ASN:HB2	1.99	0.63
1:B:231:HIS:HA	1:B:291:CYS:SG	2.38	0.63
1:A:130:ILE:C	1:A:131:ARG:HG3	2.22	0.63
1:A:205:VAL:HG13	1:A:206:PRO:HD2	1.80	0.63
1:A:475:ALA:HB1	1:A:476:PRO:HD2	1.79	0.63
1:A:195:LYS:NZ	1:A:201:PHE:O	2.33	0.62
1:A:297:ARG:HH12	1:A:328:GLU:HB3	1.63	0.62
1:B:154:LYS:HB2	1:B:154:LYS:NZ	2.14	0.62
1:B:343:GLN:HB2	1:B:478:ARG:O	1.99	0.62
1:A:383:HIS:ND1	1:A:384:LEU:N	2.37	0.62
1:B:300:LEU:HD21	1:B:334:ALA:HB2	1.81	0.62
1:A:232:THR:HG21	1:A:292:GLU:HB2	1.81	0.62
1:A:81:ALA:HB2	1:A:410:MET:HE1	1.80	0.61
1:B:185:TYR:HD1	1:B:186:SER:N	1.98	0.61
1:B:477:GLY:O	1:B:478:ARG:HG2	1.99	0.61
1:B:48:GLY:O	1:B:159:VAL:HA	2.00	0.61
1:A:124:ARG:HG3	1:B:124:ARG:HH21	1.65	0.61
1:A:47:ILE:O	1:A:103:SER:HB2	2.01	0.61
1:B:47:ILE:O	1:B:103:SER:HB2	1.99	0.61
1:B:130:ILE:C	1:B:131:ARG:HG3	2.26	0.61
1:B:463:SER:C	1:B:465:GLU:H	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HG21	1:A:253:LEU:HD21	1.82	0.61
1:B:427:MET:HE2	1:B:442:MET:CG	2.23	0.61
1:B:261:ILE:HD13	1:B:270:PHE:CE2	2.36	0.60
1:A:369:PRO:O	1:A:373:GLN:HG3	2.01	0.60
1:A:449:LYS:O	1:A:453:PHE:HB2	2.01	0.60
1:A:204:VAL:HG11	1:A:416:ALA:HA	1.84	0.60
1:A:232:THR:O	1:A:237:GLY:HA3	2.02	0.60
1:A:227:VAL:CG2	1:A:253:LEU:HD21	2.31	0.60
1:B:228:SER:OG	1:B:284:ALA:HB1	2.02	0.59
1:B:478:ARG:HH11	1:B:478:ARG:CG	2.15	0.59
1:B:425:GLN:O	1:B:428:HIS:HB3	2.03	0.59
1:B:190:ILE:HD12	1:B:208:ASP:HB2	1.85	0.59
1:B:185:TYR:CD2	1:B:413:VAL:HG22	2.38	0.58
1:A:73:GLN:H	1:A:73:GLN:NE2	2.02	0.58
1:A:293:GLY:HA3	1:A:323:ARG:NH1	2.19	0.58
1:B:201:PHE:C	1:B:201:PHE:CD2	2.82	0.58
1:B:325:GLU:OE1	1:B:325:GLU:N	2.36	0.57
1:A:185:TYR:CD2	1:A:413:VAL:HG22	2.39	0.57
1:A:231:HIS:HA	1:A:291:CYS:SG	2.44	0.57
1:B:81:ALA:HB2	1:B:410:MET:HE1	1.86	0.57
1:B:211:GLN:HE21	1:B:317:SER:HB2	1.69	0.57
1:A:261:ILE:HD13	1:A:270:PHE:CE2	2.39	0.57
1:B:335:ASN:C	1:B:335:ASN:ND2	2.62	0.57
1:B:369:PRO:O	1:B:373:GLN:HG3	2.05	0.57
1:A:228:SER:CB	1:A:287:VAL:HG22	2.31	0.57
1:B:213:ARG:HH11	1:B:247:LEU:CD2	2.18	0.57
1:A:124:ARG:HG3	1:B:124:ARG:NH2	2.20	0.57
1:B:227:VAL:CG2	1:B:253:LEU:HD21	2.35	0.56
1:A:51:PHE:HE1	1:A:185:TYR:HE2	1.53	0.56
1:A:158:GLY:HA3	1:A:420:MET:CE	2.35	0.56
1:A:185:TYR:C	1:A:185:TYR:HD1	2.14	0.56
1:B:73:GLN:H	1:B:73:GLN:NE2	2.03	0.56
1:A:185:TYR:C	1:A:185:TYR:CD1	2.84	0.56
1:A:228:SER:OG	1:A:284:ALA:HB1	2.06	0.56
1:B:380:LEU:HD23	1:B:394:CYS:HB2	1.87	0.56
1:A:301:SER:HA	1:A:330:TYR:CE2	2.40	0.56
1:A:174:LEU:HB2	1:B:177:LEU:CD1	2.36	0.56
1:A:423:GLY:HA3	1:A:454:LEU:HD23	1.86	0.56
1:A:446:ASP:CB	1:A:449:LYS:HD2	2.35	0.56
1:B:335:ASN:HA	1:B:484:LEU:HD23	1.88	0.56
1:B:489:ALA:C	1:B:491:ARG:H	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLY:C	1:A:331:GLU:H	2.14	0.55
1:A:300:LEU:HD22	1:A:334:ALA:HB2	1.87	0.55
1:B:323:ARG:CB	1:B:325:GLU:HG2	2.30	0.55
1:B:407:ASP:O	1:B:410:MET:HB3	2.06	0.55
1:B:86:LEU:O	1:B:90:ASN:ND2	2.40	0.55
1:B:335:ASN:HD21	1:B:485:GLN:HA	1.72	0.55
1:B:331:GLU:HB3	1:B:492:TYR:CD2	2.41	0.54
1:B:478:ARG:HG3	1:B:478:ARG:NH1	2.19	0.54
1:B:463:SER:O	1:B:465:GLU:N	2.40	0.54
1:A:379:ARG:O	1:A:393:VAL:HG13	2.08	0.54
1:A:325:GLU:N	1:A:325:GLU:OE1	2.40	0.53
1:A:379:ARG:HD3	1:A:390:PHE:O	2.08	0.53
1:B:373:GLN:OE1	1:B:379:ARG:HA	2.08	0.53
1:B:451:LEU:HG	1:B:452:ASP:N	2.23	0.53
1:A:446:ASP:HB3	1:A:449:LYS:HB2	1.91	0.53
1:B:270:PHE:CE1	1:B:298:GLY:HA3	2.43	0.53
1:B:495:VAL:O	1:B:497:VAL:HG13	2.09	0.53
1:A:174:LEU:HB2	1:B:177:LEU:HD13	1.90	0.53
1:B:73:GLN:HA	1:B:77:GLN:NE2	2.22	0.53
1:A:427:MET:HG2	1:A:442:MET:CE	2.39	0.53
1:B:261:ILE:HD13	1:B:270:PHE:CD2	2.43	0.53
1:B:317:SER:O	1:B:319:GLY:N	2.41	0.53
1:A:45:VAL:HG11	1:A:424:LEU:CD1	2.39	0.53
1:A:488:GLU:N	1:A:488:GLU:CD	2.67	0.53
1:A:427:MET:CE	1:A:449:LYS:HB3	2.39	0.53
1:B:119:SER:HA	1:B:122:PHE:HD2	1.74	0.52
1:A:300:LEU:HD13	1:A:334:ALA:HB2	1.90	0.52
1:B:51:PHE:HE1	1:B:185:TYR:HE2	1.55	0.52
1:A:510:TYR:CD1	1:A:510:TYR:C	2.88	0.52
1:B:368:PHE:HB3	1:B:369:PRO:CD	2.38	0.52
1:A:95:LEU:HD12	1:A:96:LEU:H	1.73	0.52
1:A:232:THR:HG21	1:A:292:GLU:OE2	2.09	0.52
1:A:339:THR:OG1	1:A:482:MET:HB2	2.09	0.52
1:B:230:VAL:O	1:B:289:CYS:HA	2.10	0.52
1:B:377:GLN:HA	1:B:390:PHE:CE2	2.44	0.52
1:A:368:PHE:HB3	1:A:369:PRO:CD	2.39	0.52
1:B:329:GLY:C	1:B:331:GLU:H	2.17	0.52
1:B:340:ILE:CG2	1:B:479:TYR:HB3	2.37	0.52
1:A:270:PHE:CE1	1:A:298:GLY:HA3	2.45	0.52
1:B:301:SER:HA	1:B:330:TYR:CE2	2.45	0.52
1:B:335:ASN:ND2	1:B:485:GLN:HA	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:CG	1:B:124:ARG:NH2	2.74	0.51
1:A:386:GLU:O	1:A:388:PRO:HD3	2.10	0.51
1:A:261:ILE:HD13	1:A:270:PHE:CD2	2.46	0.51
1:A:430:ALA:HB3	1:A:453:PHE:HZ	1.75	0.51
1:A:45:VAL:HG11	1:A:424:LEU:HD13	1.92	0.51
1:B:195:LYS:HE2	1:B:195:LYS:HA	1.92	0.51
1:B:293:GLY:HA3	1:B:323:ARG:NH1	2.25	0.51
1:A:210:LEU:O	1:A:213:ARG:HB3	2.10	0.51
1:A:383:HIS:CG	1:A:384:LEU:N	2.77	0.51
1:A:73:GLN:HA	1:A:77:GLN:NE2	2.24	0.50
1:A:373:GLN:NE2	1:A:385:LEU:O	2.44	0.50
1:B:398:GLU:OE1	1:B:398:GLU:N	2.42	0.50
1:B:57:PRO:HG3	1:B:67:CYS:HA	1.93	0.50
1:A:201:PHE:CD2	1:A:201:PHE:C	2.88	0.50
1:A:185:TYR:HD1	1:A:186:SER:N	2.09	0.50
1:A:317:SER:O	1:A:319:GLY:N	2.44	0.50
1:B:461:GLY:N	1:B:465:GLU:O	2.41	0.50
1:A:375:ARG:HG3	1:A:376:PHE:CE2	2.47	0.50
1:A:126:SER:O	1:A:130:ILE:HG12	2.12	0.50
1:B:505:LEU:HD12	1:B:506:ASN:N	2.26	0.50
1:A:190:ILE:HD11	1:A:239:SER:O	2.12	0.50
1:B:317:SER:C	1:B:319:GLY:H	2.20	0.50
1:A:47:ILE:O	1:A:103:SER:HA	2.11	0.50
1:A:202:LEU:N	1:A:202:LEU:CD2	2.70	0.50
1:B:47:ILE:HG23	1:B:420:MET:HG2	1.94	0.50
1:B:233:GLU:HB3	1:B:262:TYR:CD2	2.47	0.49
1:A:77:GLN:O	1:A:81:ALA:N	2.43	0.49
1:A:128:ILE:C	1:A:130:ILE:N	2.71	0.49
1:A:158:GLY:HA3	1:A:420:MET:HE1	1.94	0.49
1:A:119:SER:HA	1:A:122:PHE:HD2	1.75	0.49
1:A:463:SER:O	1:A:465:GLU:N	2.45	0.49
1:A:73:GLN:H	1:A:73:GLN:HE21	1.59	0.49
1:A:483:ASN:OD1	1:A:512:ILE:HG23	2.11	0.49
1:B:227:VAL:HG21	1:B:253:LEU:HD21	1.95	0.49
1:A:124:ARG:HH21	1:B:124:ARG:HG3	1.76	0.49
1:B:77:GLN:O	1:B:81:ALA:N	2.38	0.49
1:A:317:SER:C	1:A:319:GLY:H	2.21	0.49
1:A:463:SER:C	1:A:465:GLU:H	2.21	0.49
1:A:505:LEU:HD12	1:A:506:ASN:N	2.28	0.49
1:A:84:HIS:O	1:A:87:ASP:HB2	2.13	0.49
1:B:62:VAL:HB	1:B:63:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLY:HA3	1:B:420:MET:CE	2.41	0.49
1:B:169:ILE:HD12	1:B:192:LEU:HD21	1.95	0.49
1:B:339:THR:OG1	1:B:482:MET:HB2	2.12	0.49
1:B:435:HIS:CD2	1:B:439:CYS:HB3	2.47	0.49
1:A:218:ILE:HD11	1:A:481:ILE:CD1	2.34	0.49
1:A:388:PRO:O	1:A:390:PHE:N	2.46	0.49
1:A:501:HIS:C	1:A:502:GLU:HG2	2.38	0.49
1:B:126:SER:O	1:B:130:ILE:HG12	2.13	0.49
1:B:45:VAL:HG11	1:B:424:LEU:CD1	2.43	0.49
1:B:122:PHE:CD1	1:B:156:ILE:HG13	2.47	0.49
1:A:306:LEU:HG	1:A:308:VAL:HG13	1.95	0.48
1:B:99:ILE:HD11	1:B:428:HIS:CD2	2.48	0.48
1:B:427:MET:HG2	1:B:431:LEU:HD12	1.95	0.48
1:B:510:TYR:CD1	1:B:510:TYR:O	2.67	0.48
1:A:490:ASN:CG	1:A:490:ASN:O	2.55	0.48
1:A:96:LEU:N	1:A:97:PRO:HD3	2.28	0.48
1:A:407:ASP:O	1:A:410:MET:HB3	2.13	0.48
1:A:62:VAL:HB	1:A:63:PRO:HD3	1.96	0.48
1:B:213:ARG:NH1	1:B:247:LEU:HD21	2.29	0.48
1:B:478:ARG:CG	1:B:478:ARG:NH1	2.68	0.48
1:A:375:ARG:HG3	1:A:376:PHE:CD2	2.49	0.48
1:B:45:VAL:HG11	1:B:424:LEU:HD13	1.96	0.48
1:B:70:ILE:HD13	1:B:371:PHE:HB2	1.95	0.48
1:A:122:PHE:CD1	1:A:156:ILE:HG13	2.48	0.47
1:B:70:ILE:HD11	1:B:76:ILE:HD11	1.96	0.47
1:B:202:LEU:N	1:B:202:LEU:CD2	2.71	0.47
1:A:47:ILE:N	1:A:102:GLY:O	2.44	0.47
1:A:301:SER:HA	1:A:330:TYR:HE2	1.78	0.47
1:B:501:HIS:C	1:B:502:GLU:HG2	2.38	0.47
1:A:47:ILE:HG23	1:A:420:MET:HG2	1.96	0.47
1:A:190:ILE:HD13	1:A:243:ALA:HB2	1.96	0.47
1:B:221:ARG:C	1:B:222:TYR:HD2	2.22	0.47
1:B:427:MET:CG	1:B:431:LEU:HD12	2.45	0.47
1:A:192:LEU:HD22	1:A:201:PHE:CD1	2.49	0.47
1:B:195:LYS:NZ	1:B:201:PHE:O	2.48	0.47
1:A:162:PRO:HG3	1:A:171:VAL:CG2	2.40	0.47
1:B:375:ARG:HG3	1:B:376:PHE:CE2	2.50	0.47
1:A:221:ARG:C	1:A:222:TYR:HD2	2.22	0.47
1:B:477:GLY:C	1:B:478:ARG:HG2	2.40	0.47
1:B:73:GLN:H	1:B:73:GLN:HE21	1.62	0.47
1:B:124:ARG:O	1:B:128:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LYS:HB2	1:B:154:LYS:HZ2	1.79	0.46
1:A:121:GLU:OE2	1:A:124:ARG:NH2	2.47	0.46
1:A:70:ILE:HD13	1:A:371:PHE:HB2	1.97	0.46
1:A:128:ILE:O	1:A:130:ILE:N	2.45	0.46
1:A:232:THR:OG1	1:A:292:GLU:N	2.30	0.46
1:A:463:SER:C	1:A:465:GLU:N	2.73	0.46
1:A:169:ILE:HD12	1:A:192:LEU:HD21	1.97	0.46
1:B:299:LEU:O	1:B:303:MET:HG3	2.16	0.46
1:B:380:LEU:CD2	1:B:394:CYS:HB2	2.45	0.46
1:B:343:GLN:HG3	1:B:480:ASP:CG	2.41	0.46
1:A:427:MET:HA	1:A:453:PHE:CE2	2.51	0.46
1:B:190:ILE:HD11	1:B:209:THR:N	2.31	0.46
1:A:204:VAL:HG11	1:A:416:ALA:CA	2.44	0.46
1:A:500:TRP:CH2	1:A:503:GLY:N	2.83	0.46
1:B:227:VAL:HG22	1:B:253:LEU:HD21	1.97	0.46
1:B:362:ASN:HD21	1:B:365:ASN:HB3	1.81	0.46
1:B:192:LEU:HD22	1:B:201:PHE:CD1	2.51	0.46
1:B:211:GLN:NE2	1:B:317:SER:HB2	2.30	0.46
1:A:47:ILE:HD12	1:A:86:LEU:HD21	1.97	0.46
1:A:402:GLU:O	1:A:402:GLU:HG3	2.16	0.46
1:A:479:TYR:HB2	1:A:500:TRP:HB3	1.97	0.46
1:B:424:LEU:HD23	1:B:450:LEU:HD13	1.97	0.46
1:B:332:VAL:HG23	1:B:333:GLU:N	2.31	0.45
1:A:361:THR:O	1:A:363:THR:HG23	2.15	0.45
1:B:205:VAL:HG23	1:B:342:LEU:HD21	1.98	0.45
1:B:231:HIS:HB3	1:B:241:MET:HE2	1.97	0.45
1:A:335:ASN:ND2	1:A:492:TYR:CE1	2.84	0.45
1:B:454:LEU:O	1:B:457:SER:HB2	2.15	0.45
1:B:98:ASN:HB2	1:B:436:VAL:HG12	1.97	0.45
1:A:231:HIS:HB3	1:A:241:MET:HE2	1.99	0.45
1:B:185:TYR:CE2	1:B:413:VAL:HG22	2.52	0.45
1:B:270:PHE:O	1:B:273:LEU:HB3	2.17	0.45
1:A:188:THR:HG22	1:A:206:PRO:O	2.17	0.45
1:A:296:VAL:O	1:A:299:LEU:N	2.50	0.45
1:B:317:SER:C	1:B:319:GLY:N	2.75	0.45
1:B:489:ALA:C	1:B:491:ARG:N	2.75	0.45
1:A:239:SER:OG	1:A:240:GLY:N	2.49	0.45
1:A:433:PRO:C	1:A:435:HIS:H	2.24	0.45
1:A:461:GLY:HA3	1:A:465:GLU:CG	2.45	0.45
1:A:427:MET:HE1	1:A:449:LYS:CB	2.46	0.45
1:B:508:ASP:OD1	1:B:510:TYR:CD2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:SER:HA	1:A:467:VAL:O	2.16	0.45
1:A:495:VAL:O	1:A:497:VAL:HG13	2.16	0.45
1:B:84:HIS:O	1:B:87:ASP:HB2	2.16	0.45
1:A:70:ILE:HD11	1:A:76:ILE:HD11	1.99	0.44
1:A:343:GLN:HE21	1:A:343:GLN:HB2	1.47	0.44
1:B:301:SER:HA	1:B:330:TYR:HE2	1.82	0.44
1:B:332:VAL:HG23	1:B:333:GLU:H	1.82	0.44
1:B:483:ASN:OD1	1:B:512:ILE:HG23	2.17	0.44
1:A:82:MET:HA	1:A:417:ILE:CD1	2.47	0.44
1:A:425:GLN:O	1:A:428:HIS:HB3	2.16	0.44
1:A:308:VAL:C	1:A:309:VAL:HG23	2.43	0.44
1:B:190:ILE:CD1	1:B:208:ASP:HB2	2.46	0.44
1:A:130:ILE:HG22	1:A:130:ILE:O	2.17	0.44
1:A:343:GLN:NE2	1:A:478:ARG:HB3	2.31	0.44
1:A:205:VAL:HG13	1:A:206:PRO:CD	2.45	0.44
1:A:359:LEU:HD11	1:A:369:PRO:HA	2.00	0.44
1:A:124:ARG:O	1:A:128:ILE:HG12	2.17	0.44
1:A:204:VAL:CG1	1:A:416:ALA:HA	2.46	0.44
1:A:355:LEU:C	1:A:357:LEU:H	2.26	0.44
1:B:320:TRP:O	1:B:323:ARG:HG3	2.18	0.44
1:B:358:ARG:HH11	1:B:358:ARG:CG	2.28	0.44
1:A:283:LYS:C	1:A:285:ARG:H	2.25	0.44
1:A:190:ILE:CG2	1:A:209:THR:H	2.30	0.43
1:A:287:VAL:HB	1:A:314:LEU:HD23	1.99	0.43
1:B:341:LYS:HG2	1:B:342:LEU:N	2.33	0.43
1:A:124:ARG:CG	1:B:124:ARG:HH21	2.31	0.43
1:A:300:LEU:HD21	1:A:334:ALA:HB2	1.95	0.43
1:B:130:ILE:O	1:B:130:ILE:HG22	2.18	0.43
1:B:158:GLY:HA3	1:B:420:MET:HE1	1.99	0.43
1:B:211:GLN:NE2	1:B:318:ASP:OD1	2.49	0.43
1:B:236:TYR:CE2	1:B:290:PHE:CD2	3.06	0.43
1:A:195:LYS:HA	1:A:195:LYS:HE2	2.01	0.43
1:B:55:HIS:ND1	1:B:71:ARG:HD2	2.33	0.43
1:B:218:ILE:HD11	1:B:481:ILE:HG23	2.00	0.43
1:A:154:LYS:HG2	1:A:155:PRO:HD2	2.00	0.43
1:A:73:GLN:HE21	1:A:73:GLN:HB2	1.54	0.43
1:A:84:HIS:HB2	1:A:353:TYR:CE2	2.54	0.43
1:A:373:GLN:OE1	1:A:380:LEU:HG	2.18	0.43
1:B:82:MET:HA	1:B:417:ILE:CD1	2.49	0.43
1:B:449:LYS:O	1:B:453:PHE:HB2	2.19	0.43
1:A:54:HIS:O	1:A:109:CYS:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLU:OE1	1:A:398:GLU:N	2.38	0.43
1:B:205:VAL:CG2	1:B:342:LEU:HD21	2.48	0.43
1:B:378:CYS:C	1:B:394:CYS:SG	3.02	0.43
1:B:427:MET:HE1	1:B:445:ILE:HG23	2.00	0.43
1:A:169:ILE:HG22	1:A:170:GLN:N	2.33	0.43
1:A:185:TYR:CE2	1:A:413:VAL:HG22	2.53	0.43
1:A:124:ARG:NH2	1:B:124:ARG:HG3	2.33	0.42
1:A:233:GLU:HB3	1:A:262:TYR:CE2	2.54	0.42
1:A:317:SER:C	1:A:319:GLY:N	2.76	0.42
1:A:451:LEU:HG	1:A:452:ASP:N	2.33	0.42
1:B:380:LEU:O	1:B:386:GLU:HG3	2.19	0.42
1:A:47:ILE:O	1:A:103:SER:CB	2.66	0.42
1:A:285:ARG:HH11	1:A:285:ARG:HG3	1.83	0.42
1:B:221:ARG:HE	1:B:221:ARG:HB2	1.64	0.42
1:B:331:GLU:HG2	1:B:492:TYR:HB2	2.02	0.42
1:A:240:GLY:HA3	1:A:290:PHE:CE1	2.54	0.42
1:A:262:TYR:HD2	1:A:262:TYR:HA	1.74	0.42
1:B:47:ILE:HD12	1:B:86:LEU:HD21	2.01	0.42
1:B:122:PHE:HD1	1:B:156:ILE:HG13	1.84	0.42
1:B:185:TYR:O	1:B:205:VAL:HG11	2.19	0.42
1:A:270:PHE:O	1:A:273:LEU:HB3	2.20	0.42
1:A:306:LEU:HG	1:A:306:LEU:O	2.20	0.42
1:A:328:GLU:O	1:A:330:TYR:HD1	2.02	0.42
1:B:241:MET:HG3	1:B:245:LYS:HG3	2.00	0.42
1:A:358:ARG:NH1	1:A:358:ARG:HG2	2.34	0.42
1:B:47:ILE:N	1:B:102:GLY:O	2.49	0.42
1:B:185:TYR:CD1	1:B:186:SER:N	2.83	0.42
1:A:423:GLY:HA3	1:A:454:LEU:CD2	2.48	0.42
1:B:294:MET:HE2	2:B:704:SO4:O4	2.20	0.42
1:A:354:PHE:O	1:A:354:PHE:CG	2.72	0.42
1:B:84:HIS:HB2	1:B:353:TYR:CE2	2.55	0.42
1:A:173:ASN:HD22	1:A:173:ASN:HA	1.74	0.42
1:B:192:LEU:HD22	1:B:201:PHE:CG	2.54	0.42
1:B:358:ARG:HG2	1:B:358:ARG:NH1	2.30	0.42
1:A:308:VAL:O	1:A:309:VAL:CG2	2.68	0.42
1:A:119:SER:O	1:A:122:PHE:HB2	2.20	0.42
1:B:328:GLU:O	1:B:330:TYR:HD1	2.02	0.41
1:A:124:ARG:NH2	1:B:124:ARG:CG	2.83	0.41
1:A:500:TRP:CZ3	1:A:502:GLU:HA	2.55	0.41
1:B:47:ILE:O	1:B:103:SER:HA	2.19	0.41
1:B:108:SER:C	1:B:110:TRP:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ASN:ND2	1:B:336:GLY:N	2.68	0.41
1:A:446:ASP:OD1	1:A:446:ASP:C	2.63	0.41
1:B:232:THR:O	1:B:237:GLY:HA3	2.20	0.41
1:B:387:ASN:OD1	1:B:389:ASN:N	2.50	0.41
1:A:117:GLU:HG3	1:B:127:LEU:HD13	2.03	0.41
1:A:368:PHE:CB	1:A:369:PRO:HD3	2.45	0.41
1:A:407:ASP:CB	1:A:410:MET:HB2	2.35	0.41
1:B:287:VAL:HB	1:B:314:LEU:HD23	2.02	0.41
1:B:331:GLU:O	1:B:335:ASN:HB2	2.20	0.41
1:B:379:ARG:HB3	1:B:387:ASN:O	2.20	0.41
1:A:335:ASN:ND2	1:A:492:TYR:HE1	2.17	0.41
1:A:206:PRO:HB3	1:A:477:GLY:HA2	2.03	0.41
1:B:154:LYS:HG2	1:B:155:PRO:HD2	2.03	0.41
1:B:188:THR:HG22	1:B:206:PRO:O	2.20	0.41
1:B:296:VAL:O	1:B:299:LEU:N	2.52	0.41
1:B:459:PHE:CZ	1:B:467:VAL:HG11	2.55	0.41
1:A:84:HIS:HB2	1:A:353:TYR:CD2	2.56	0.41
1:B:214:ALA:HA	1:B:500:TRP:NE1	2.35	0.41
1:B:435:HIS:CD2	1:B:439:CYS:CB	3.04	0.41
1:A:169:ILE:CD1	1:A:192:LEU:HG	2.51	0.41
1:B:188:THR:HA	1:B:203:ARG:NH1	2.36	0.41
1:B:303:MET:HE3	1:B:312:PHE:HD2	1.85	0.41
1:B:343:GLN:HG3	1:B:480:ASP:OD2	2.21	0.41
1:B:384:LEU:H	1:B:384:LEU:HG	1.66	0.41
1:A:329:GLY:C	1:A:331:GLU:N	2.79	0.41
1:A:407:ASP:OD2	1:A:408:SER:N	2.54	0.41
1:A:408:SER:C	1:A:410:MET:H	2.29	0.41
1:B:208:ASP:O	1:B:211:GLN:HB2	2.20	0.41
1:B:169:ILE:CD1	1:B:192:LEU:HG	2.50	0.40
1:B:418:TYR:O	1:B:421:ALA:HB3	2.21	0.40
1:B:56:GLN:HA	1:B:57:PRO:HD3	1.95	0.40
1:A:179:ASP:HA	1:A:200:TYR:CE2	2.56	0.40
1:A:192:LEU:HD22	1:A:201:PHE:CG	2.56	0.40
1:A:315:ILE:HA	1:A:338:ILE:O	2.21	0.40
1:A:323:ARG:CB	1:A:325:GLU:HG2	2.35	0.40
1:B:222:TYR:N	1:B:222:TYR:CD2	2.87	0.40
1:B:222:TYR:HD1	1:B:224:TRP:CH2	2.38	0.40
1:B:236:TYR:CZ	1:B:290:PHE:HE2	2.40	0.40
1:B:355:LEU:C	1:B:357:LEU:H	2.28	0.40
1:B:236:TYR:CD2	1:B:236:TYR:C	2.99	0.40
1:B:305:ARG:C	1:B:307:GLY:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:HG11	1:A:332:VAL:HG12	2.03	0.40
1:A:355:LEU:HD22	1:A:401:GLU:CG	2.49	0.40
1:B:236:TYR:CE2	1:B:290:PHE:CE2	3.10	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	452/490 (92%)	391 (86%)	55 (12%)	6 (1%)	9	38
1	B	452/490 (92%)	397 (88%)	47 (10%)	8 (2%)	6	34
All	All	904/980 (92%)	788 (87%)	102 (11%)	14 (2%)	8	36

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ALA
1	A	389	ASN
1	B	256	ALA
1	A	318	ASP
1	A	330	TYR
1	A	440	ASP
1	B	318	ASP
1	B	440	ASP
1	B	508	ASP
1	A	129	SER
1	B	490	ASN
1	B	502	GLU
1	B	330	TYR
1	B	447	GLY

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	392/422 (93%)	364 (93%)	28 (7%)	13	40
1	B	392/422 (93%)	354 (90%)	38 (10%)	8	31
All	All	784/844 (93%)	718 (92%)	66 (8%)	10	35

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	73	GLN
1	A	82	MET
1	A	94	VAL
1	A	154	LYS
1	A	155	PRO
1	A	169	ILE
1	A	185	TYR
1	A	188	THR
1	A	190	ILE
1	A	197	LEU
1	A	202	LEU
1	A	205	VAL
1	A	209	THR
1	A	233	GLU
1	A	242	ASP
1	A	247	LEU
1	A	262	TYR
1	A	289	CYS
1	A	313	SER
1	A	325	GLU
1	A	333	GLU
1	A	342	LEU
1	A	399	SER
1	A	453	PHE
1	A	495	VAL
1	A	497	VAL

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Mol	Chain	Res	Type
1	A	508	ASP
1	B	37	SER
1	B	41	MET
1	B	73	GLN
1	B	82	MET
1	B	95	LEU
1	B	126	SER
1	B	129	SER
1	B	154	LYS
1	B	155	PRO
1	B	169	ILE
1	B	185	TYR
1	B	188	THR
1	B	190	ILE
1	B	197	LEU
1	B	202	LEU
1	B	204	VAL
1	B	210	LEU
1	B	211	GLN
1	B	242	ASP
1	B	247	LEU
1	B	262	TYR
1	B	289	CYS
1	B	294	MET
1	B	324	ASP
1	B	325	GLU
1	B	335	ASN
1	B	343	GLN
1	B	377	GLN
1	B	379	ARG
1	B	384	LEU
1	B	397	ASN
1	B	399	SER
1	B	453	PHE
1	B	487	THR
1	B	493	ASP
1	B	495	VAL
1	B	497	VAL
1	B	510	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	77	GLN
1	A	173	ASN
1	A	176	GLN
1	A	250	GLN
1	A	257	HIS
1	A	264	ASN
1	A	343	GLN
1	A	362	ASN
1	A	374	HIS
1	A	429	HIS
1	A	501	HIS
1	A	506	ASN
1	B	73	GLN
1	B	173	ASN
1	B	211	GLN
1	B	250	GLN
1	B	257	HIS
1	B	264	ASN
1	B	335	ASN
1	B	343	GLN
1	B	362	ASN
1	B	374	HIS
1	B	429	HIS
1	B	435	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 ⓘ

5 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	A	701	-	4,4,4	0.39	0	6,6,6	0.23	0
2	SO4	B	703	-	4,4,4	0.36	0	6,6,6	0.17	0
3	NAG	B	601	1	14,14,15	0.88	0	17,19,21	0.85	0
2	SO4	B	704	-	4,4,4	0.37	0	6,6,6	0.18	0
2	SO4	A	702	-	4,4,4	0.36	0	6,6,6	0.24	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	NAG	B	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	NAG	O5-C5-C6-O6
3	B	601	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	NAG	1	0
2	B	704	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	456/490 (93%)	-0.28	2 (0%) 88 72	32, 69, 110, 123	0
1	B	456/490 (93%)	-0.28	1 (0%) 91 80	31, 68, 112, 124	0
All	All	912/980 (93%)	-0.28	3 (0%) 90 76	31, 69, 112, 124	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	490	ASN	2.2
1	B	223	ASN	2.1
1	A	510	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
3	NAG	B	601	14/15	0.55	0.14	93,96,100,101	0
2	SO4	B	704	5/5	0.72	0.10	92,92,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	703	5/5	0.88	0.11	88,89,89,90	0
2	SO4	A	701	5/5	0.91	0.08	81,82,83,83	0
2	SO4	A	702	5/5	0.92	0.07	72,73,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.